

Fixed Scale Transformation Approach for Born Model of Fractures.

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Abstract

We use the Fixed Scale Transformation theoretical approach to study the problem of fractal growth in fractures generated by using the Born Model. In this case the application of the method is more complex because of the vectorial nature of the model considered. In particular, one needs of a careful choice of the lattice path integral for the fracture evolution and the identification of the appropriate way to take effectively into account screening effects. The good agreement of our results with computer simulations shows the validity and flexibility of the FST method in the study of fractal patterns evolution.

The study of fractal growth models is an important field of the modern statistical mechanics that attempts to understand the origin and evolution of many examples of fractal structures observed in nature. One of the most familiar events in which one observes the formation of fractal patterns is the mechanical breakdown. In this work we shall modelize fractures according to the Born Model (BM) [1, 2] In the BM there are two contributions to the energy of the medium V to take into account the classical behaviour of a $2 - d$ network of elastic springs, that is

$$\begin{aligned}
 V &= \frac{1}{2} \sum_{i,j} V_{ij} = \\
 &= \frac{1}{2}(\alpha - \beta) \sum_{i,j} [(\vec{u}_i - \vec{u}_j) \cdot \hat{r}_{ij}]^2 + \frac{1}{2}\beta \sum_{i,j} [\vec{u}_i - \vec{u}_j]^2
 \end{aligned} \tag{1}$$

where \vec{u}_i is the displacement vector of site i , \hat{r}_{ij} is the unit vector between i and j , α and β are force constants (keeping α fixed, one can tune the model only varying the value of the other parameter β) and the sum runs over nearest neighbors sites. In this model the formation of cracks is probabilistic: it is obtained through an iterative addition of broken lattice bonds to the fracture already grown. At every step the new broken bond is chosen as follows:

- one minimizes the energy of the lattice, i.e. eq. (1) with respect to the displacement field \vec{u}_i ;
- a new bond to break is chosen on the surface of crack with probability:

$$p_{ij} = \frac{V_{ij}^{\frac{\eta}{2}}}{\sum_{ij} V_{ij}^{\frac{\eta}{2}}} \tag{2}$$

where η is a free parameter of the model;

The relations that one has between the \vec{u}_i minimizing eq. (1) are formally very similar to those between scalar fields in the processes of growth driven by a Laplacian operator. Then one can say that BM has an analogy with other models of fractal growth as the Dielectric Breakdown Model (DBM)[3] and Diffusion Limited Aggregation (DLA)[4] for Laplacian growth, describing very simply the fracture propagation controlled by growth instabilities and allowing us to take into account the vectorial nature of the problem.

There are some numerical simulations[2, 5], from which it is clear the dependence of the value of fractal dimension on the parameters of the model. That is, increasing the value of η there is a reduction of the fractal dimension. The same effect can be obtained by tuning

the ratio $\frac{\beta}{\alpha}$ that measures the weight of the two different kinds of contribution at the energy of the system. For instance, a typical value for $\eta = 1$, $\beta = 0$, $\alpha = 1$ is $D = 1.52 \pm 0.04$. One example of the kind of patterns obtained is in Fig.1

A crucial point in the study of fractures is the lack of a theoretical framework in which to study the evolution of the fractal patterns. For this reason we want to extend a method called Fixed Scale Transformation (FST) [6, 7] to the study of the mechanical breakdown.

The Fixed Scale Transformation is a theoretical scheme that allows to address the problem of a systematic calculation of the fractal dimension and other scaling properties for a wide range of irreversible growth models. The basic point of the FST method is to treat separately the asymptotic time limit ($t \rightarrow \infty$) and the large scale limit $b \rightarrow \infty$. The method starts by considering the problem of the asymptotic time limit and defining the nearest neighbour(n-n) pair correlations at a generic scale using lattice path integrals calculation method. Then, using in the calculation the scale invariant growth rules of the models, it is possible to characterize the asymptotic correlation properties $b \rightarrow \infty$ for coarse grained variables, obtaining finally the fractal dimension. Analyzing the asymptotic dynamics, it can be shown that the minimal scale growth rules of these models can be considered as a good approximation to the asymptotic one [8, 9]. A detailed discussion of the FST method can be found in ref [10].

The previous n-n pair correlations at a generic scale can be computed considering the transverse correlation along the intersection of the structure with a line perpendicular to the local growth direction. In two dimension, since we are interested in conditional probabilities, there are two types of pair configurations in the asymptotic structures. A configuration of type 1 consisting of an occupied site and an empty one, and a type 2 with both sites occupied. The probabilities of these configurations are defined as C_1 and C_2 respectively. In order to compute these probabilities it is convenient to consider the probability $M_{i,j}$ that a pair configuration of type i is followed in the growth direction by a configuration of type j . These conditional probabilities are defined by the lattice path integrals corresponding to the various growth process and it leads us to a transfer matrix problem. If k is the iteration order one has:

$$\vec{C}^k = M\vec{C}^{k-1}, \quad (3)$$

where

$$M = \begin{pmatrix} M_{11} & M_{21} \\ M_{12} & M_{22} \end{pmatrix}$$

From the FST given by Eq.3 one obtains, in the limit $k \rightarrow \infty$, the fixed point probabilities (C_1, C_2) that, in principle, characterize only the nearest neighbours correlations at the minimal scale. However, were it possible to interpret our sites as coarse grained cells and use

growth rules that are scale invariant, then the fixed point probabilities would characterize the correlations between coarse grained cells of any size. In such a situation our pairs of cells of variable sizes can be shown to correspond to the box covering process of an intersection of the structure with a line perpendicular to the growth direction. In this way the probability distribution (C_1, C_2) can be related to the fractal dimension of the structure

$$D = 1 + \frac{\ln(C_1 + 2C_2)}{\ln 2}. \quad (4)$$

We start with a configuration of type i and then we consider a growth column above it [6]. The matrix elements are evaluated by summing up the weight of each graph of a given order (number of growth processes considered that lead from a configuration of type i to a configuration of type j).

Because of the screening effects present in these kinds of fractal growth phenomena, one has a rapid convergence of the value of the matrix element. This allow to study only few step of the growth, that is to consider only graphs of a small order.

In the case of fracture propagation the main problem is the definition of the diagrammatical technique, that is which are the basic configuration and how to determine the possible path in the evolution. It is clear that one can not study simply the state of sites, but has to deal with all the bond connecting the site. Furthermore, the use of small cells such as those used for the DLA case induce in the calculation serious small size effects. In fact, on a triangular network the behavior expected is a fracture orthogonal to the external strain direction. For small cells however, the growth is composed by successive steps in which the horizontal bonds, the most stressed, are always broken. This effect is intrinsic to the model in which, at the scale of a small cell computation, the correct growth behavior is mixed with a bias due to the underlying triangular lattice.

Thus, the kind of microscopic structure of the model does not allow a small cell treatment of the problem, and to address the evolution in the usual scheme of the FST approach, one needs of an enlarged space of configurations and an enlarged growth column [11]. This results in a dramatic computational complexity and for these reasons we have chosen a different geometry for the growth column and the set of bond configurations shown in Fig.2 and Fig.3. This changes remarkably the usual FST diagrammatic technique, but allows us to take into account the vectorial nature of the problem.

We call a configuration of kind C_2 only in the case shown in Fig. 3, using the horizontal bonds as carrier of the fracture for the superior cells. The price to pay for this simplification is that now the evolution of these bonds does not affect the value of the fractal dimension. Removing an horizontal bond does not change the matrix elements and one has to go on the next order of calculation. For this reason one needs to go until the sixth order in the

probability tree to have stable results.

In order to perform the enumeration of the growth configurations, the simplest choice, is to study the growth only in a column of two-site cells. An approximate scheme to describe the presence of external cracks is to consider two opposite situation, one called “open boundary condition” in which there are not sites occupied around the column; the second called “closed boundary condition”. In the second the lattice on which the pattern is grown is made by replicas of the column studied and this is done to make possible all the processes of growth from outside described before.

For the exact enumeration of the various configurations we have used an algorithm which starts from replicas of C_1 configurations in the middle of lattice. We then analyzed the probability tree of all the possible paths (for the first order is in Fig.4, for the higher orders one has to break more bonds). The statistical weight of each path is therefore given by the product of the probability of each elementary growth process in the growth column. Depending on the initial and final configuration, this weight contributes to the definition of one of the M_{ij} (it is the sum over all possible path from configuration i to j). With these matrix elements it is finally possible to compute the value of the fractal dimension. In columns “**OP.**” of Tab.1 we show the results. It is evident how the behaviour of the fractal dimension value depends strongly on the ratio $\frac{\beta}{\alpha}$.

For the closed boundary condition, we have done a similar work and we have obtained the values in the second part of Tab.1, the respective probability tree is in Fig.5.

In analogy with the DLA model we have used for the calculation of the fractal dimension the first non-trivial scheme that includes self-consistently the fluctuations of the boundary conditions. This scheme is called the open-closed approximation [11] and it is possible in this case to derive analytically the fixed point distribution (C_1, C_2) . In this way one obtains the final value of Tab.2 in which is to be noticed the high order necessary to reach a good convergency of the results as explained before.

In the case of $\beta = 0$ the results, can be directly compared with Montecarlo results. The good agreement of this value (1.52 versus 1.56) is a good test of the validity of this approach also for patterns obtained in the evolution of a vectorial field. In this case in fact the value of the fractal dimension shows a good convergency as a function of the order of calculation. Unfortunately for the case $\beta \neq 0$ one has a less satisfactory convergence towards a limiting value. Because of the dramatic proliferation of the configurations it was not possible to reach a higher order of approximation for larger values of β . It has to be noticed, anyway, that when the convergence is reached, also for small values of β , one has again a satisfying prevision of the model behaviour as in the case of $\beta = 0.1$. In fact, we find here a value of the fractal dimension $D = 1.648$ versus a value of $D = 1.68$.

In conclusion the extension of the FST to the BM case is conceptually straightforward and can be done along the line of the DLA calculation. In practice however, the new nature of the growth dynamics makes the treatment substantially more complex. Nevertheless, the FST method can be extended in a natural way to this problem and the results obtained are in good agreement with those obtained from computer simulations. This is therefore an important test for the validity of the FST as a general analytical tool to study irreversible fractal growth phenomena introducing the appropriate theoretical perspective in this field.

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$\beta =$	0		0.1		0.8	
order	OP.	CL.	OP.	CL.	OP.	CL.
3	1.354	1.504	1.429	1.283	1.407	1.120
4	1.436	1.506	1.614	1.396	1.575	1.184
5	1.575	1.507	1.763	1.420	1.700	1.211
6	1.585	1.507	1.813	1.462	1.766	1.243
7	-	-	1.854	1.480	-	-

D IN <i>OPEN-CLOSED</i> APPR.			
$\beta =$	0	0.1	0.8
order			
3	1.385	1.393	1.350
4	1.452	1.533	1.475
5	1.555	1.611	1.534
6	1.560	1.645	1.571
7	-	1.648	-

Table Captions

1. Values of fractal dimensions for open boundary condition and closed boundary condition, for different β values. In the case of $\beta = 0.8$ there is a not complete convergence.
2. Values of fractal dimensions in the open closed approximation, for the same value of β used in Tab.1. In the case of $\beta = 0.8$ there is a not complete convergence.

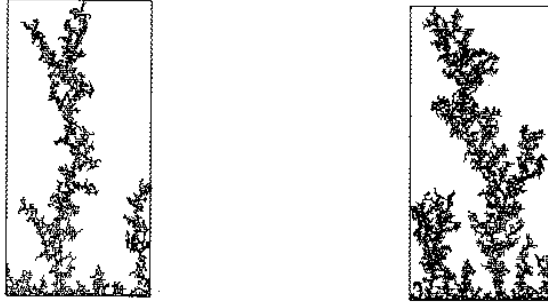


Figure 1: Some typical fractures produced by computer simulation using the Born Model. In the case a) $\alpha = 1$, $\beta = 0$ and $\eta = 0.8$, in the case b) $\alpha = 1$, $\beta = 0.5$ and $\eta = 1$. The colour of pattern changes with the fracture growth.

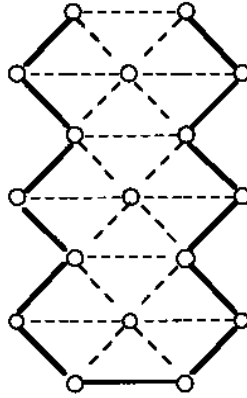


Figure 2: The new column of growth composed by bonds.

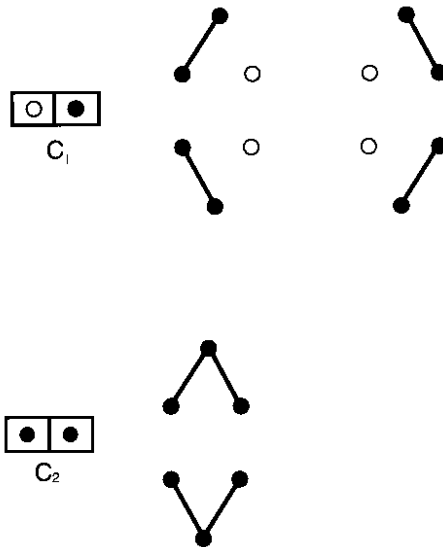


Figure 3: The new definitions for the basic configurations C_1 and C_2 .

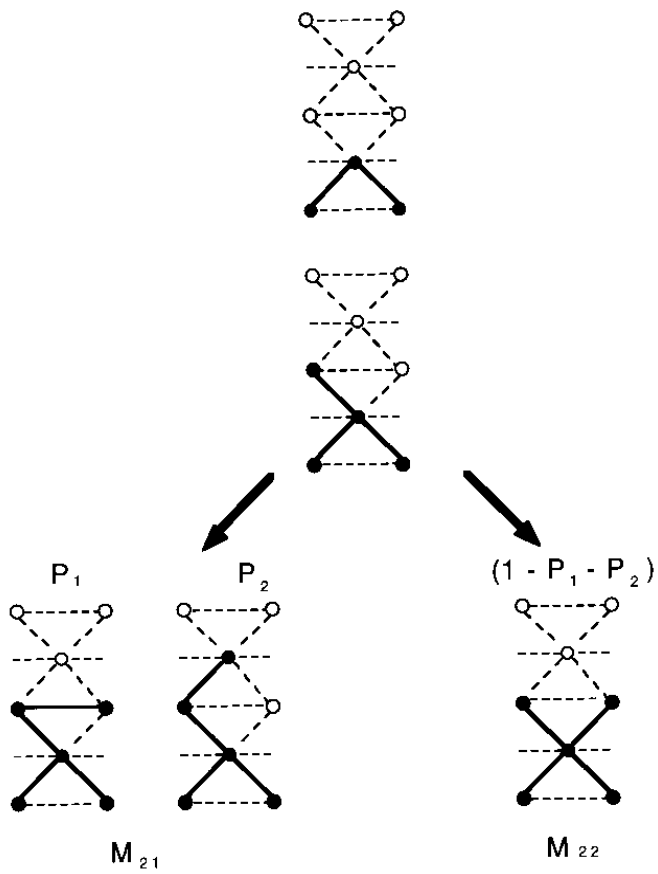


Figure 4: Probability tree at the first order for the computation of matrix elements in open boundary conditions.

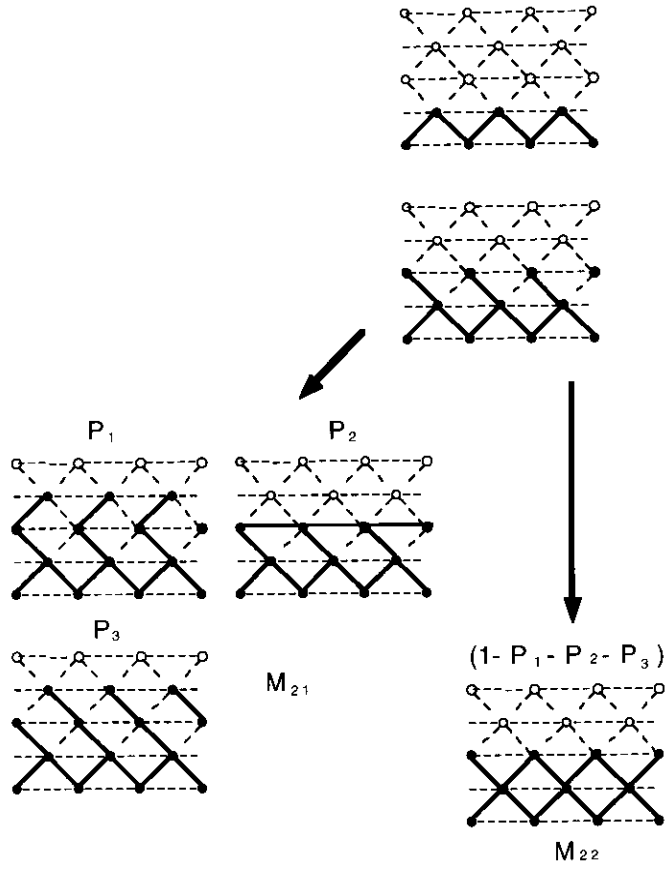


Figure 5: Probability tree at the first order for the computation of matrix elements in closed boundary conditions.