Fractal dimension of collision cascades

F. Kun* and G. Bardos
Department of Theoretical Physics, Kossuth Lajos University, P.O. Box 5, H-4010 Debrecen, Hungary
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The geometrical structure of the vacancy distribution in collision cascades is studied using Monte Carlo simulations. Based on a Flory–de Gennes-type approach, a relation of the fractal dimension, the self-similarity dimension, and the dimension of the embedding space is established. It is shown that, varying the parameter of the interaction potential, a structural transition takes place in the cascade from an open branching structure to a space-filling one. Based on the results the spike condition of Cheng, Nicolet, and Johnson [Phys. Rev. Lett. 58, 2083 (1987)] is revisited. [S1063-651X(97)12602-2]

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I. INTRODUCTION

Collision cascades develop in condensed matter as a consequence of irradiation with energetic beams of particles. The bombarding particles transfer their kinetic energy in series of collisions with the target atoms and the energized, recoiling atoms generate further recoils in their own slowing-down process. The result of this energy sharing process is a collision cascade.

To study the geometrical structure of collision cascades there are two possible viewpoints: On the one hand, the cascade can be considered as a treelike geometrical object, which is composed of the trajectories of the moving particles and points where the collisions occurred [1,2]. Recently we showed that in this consideration the cascade-tree exhibits multiscaling and multifractality, which is a direct consequence of the underlying multiplicative process of the cascade mechanism [3].

On the other hand, the cascade can be treated as a branched aggregate of the vacancies created in sequential collisions during the cascade evolution. This vacancy distribution in the target is bounded by the interstitials, making this damaged region in the solid well defined. Randomly branched aggregates occur in many physical systems such as branched polymers, the sol-gel transition, percolation, turbulence, nucleation, the formation of smoke particles, and electric breakdown. The common feature of these objects is that they all show a strong degree of self-similarity [4]. From the geometrical point of view the structure of the vacancy distribution in the collision cascades is analogous to the structure of randomly branched aggregates.

Recently vacancy distribution in collision cascades has been investigated from the viewpoint of fractal geometry by means of analytical calculations and of Monte Carlo (MC) simulations in the framework of the binary collision approximation (BCA). These investigations have been extended to the study of the self-similarity properties of the cascade [5,6], to the determination of its fractal dimension for different interaction potentials [1–3,7,8], and to the study of cascade-subcascade transition and spikes [5,8]. A simple deterministic fractal-tree model (see Fig. 1) was proposed [5] as an average cascade for the case of an inverse-power potential of the type

$$V(r)=G(m)r^{-1/m}, \quad 0<m\leqslant 1. \tag{1}$$

It was shown that the self-similarity dimension of the deterministic tree $D_0(m)=1/2m$ in $d=3$ embedding Euclidean space. It depends solely on the parameter m of the interaction potential. To test the predictions of this model, MC simulations were performed. It was found that the measured (MC)

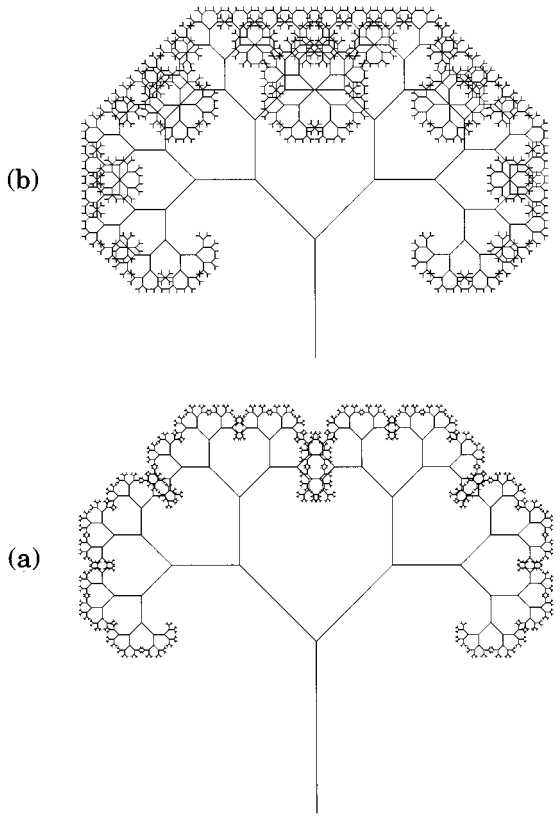

FIG. 1. Deterministic cascade trees up to ten generation steps with different similarity ratios γ. (γ is the ratio of two successive branches in the tree.) (a) $\gamma=0.6$. (b) $\gamma=0.7$. One can observe that for increasing γ (decreasing m) the overlap of different branches is increasing.

*Electronic address: feri@dtp.atomki.hu

fractal dimension $D(m)$ of the vacancy distribution is in good agreement with the self-similarity dimension $D_0(m)$ only in the range $m>\frac{1}{3}$. If $m\leqslant\frac{1}{3}$, then $D(m)<D_0(m)$, and the difference of these two dimensions increases as m goes to zero [1,2,7,8]. This so called nonlinearity of damage production is due to the overlapping effect of subcascades.

To make this situation more clear we performed systematic MC studies in $d=2$ $(2d)$ and $d=3$ $(3d)$ embedding dimensions in a wide range of the parameter of the potential m. In the present paper we clarify the connection of the measured fractal dimension D of the cascade, the self-similarity dimension D_0 of the deterministic model, and the Euclidean dimension d of the embedding space. Based on a Flory–de Gennes-type mean-field approach [9,10] for the fractal dimension, we have established an explicit relation of the type $D=D(D_0,d)$. The predictions of our expression $D=D(D_0,d)$ is in a good agreement with the fractal dimension extracted from the MC data.

We note that there are differences between the reasons of the applicability of the Flory – de Gennes arguments in the study of cascades and in the study of the other type of branching aggregates. In the case of polymers and diffusion-limited aggregates, the excluded volume effect as a geometrical constraint causes geometrical correlations in the systems, and this can affect the actual structure, increasing the radius of gyration and decreasing the fractal dimension [9–15]. But in the simulation of collision cascades the target was supposed to be amorphous; furthermore, there was no restriction for the distance of the vacancies belonging to different branches of the cascade, and the vacancies forming the cascade were supposed to be pointlike objects. It follows that there was no excluded volume effect included in our simulations. In the cascades geometrical correlations arise from other reasons, namely, because of the overlapping of the subcascades.

Recently, based on a Flory-type theory, Family pointed out [11] that the random branching fractals can have only three possible equilibrium shapes in the presence of geometrical correlation, and he classified these objects into extended, compensated, and collapsed states. It is shown in the present paper that decreasing the parameter of the potential m from 1 toward 0, the system goes through these states of the evolution. Thus varying m as a control parameter a transition takes place in the cascade from an open-branching structure toward a compact shape, the fractal dimension being equal to the dimension of the embedding space.

The outline of the remainder of this paper is as follows. In Sec. II, the construction of the deterministic cascade model, the concept of the self-similarity dimension and fractal dimension is briefly reviewed, and numerical results are presented for the fractal dimension of the vacancy distribution. We compare the fractal dimensions obtained numerically to the corresponding self-similarity dimensions. To understand the reason of the discrepancy between them in Sec. III. a Flory–de Gennes-type mean-field approach is established, and at the end the spike condition of Ref. [5] is revisited.

II. SELF-SIMILARITY DIMENSION, FRACTAL DIMENSION

In a self-ion collision cascade, where the projectile and the target atoms are the same, the scattering angle falls between 0 and $\pi/2$. The geometrical model of self-ion collisional cascades was established by Cheng, Nicolet, and Johnson as an average cascade for the case of the interaction potential Eq. (1). This model is a deterministic one, which is constructed by allowing the single value $\pi/4$ of the scattering angle solely for all the collisional generations (Fig. 1). This way a so-called fractal tree is constructed which is rigorously self-similar up to the scale of the entire system, with the similarity ratio γ being the ratio of two successive branches in the tree. This construction is based on the fact that in the hard sphere approximation of the scattering process the expectation value of the particle energy (scattered and recoiled) is given by $\overline{E}=1/2E$ (which belongs to the $\pi/4$ scattering angle) and the mean free-flight path L_{kv} between two successive collisions has the simple energy dependence $L_{kv}=KE^{2m}$ (K is energy independent). Thus the average cascade might be substituted by a deterministic one, with the similarity ratio $\gamma=(1/2)^{2m}$ being the ratio of two successive branches at the scattering angle $\pi/4$ [5].

Let us suppose that $N(r)$ boxes of size r are required to cover this deterministic tree in the d-dimensional embedding space. Changing the scale of the observation to γr, $N(\gamma r)$ boxes are needed to cover the object. Because of the self-similarity we obtain

$$N(\gamma r)=2N(r)=\gamma^{-D_0}N(r). \tag{2}$$

This means that $N(r)$ is a homogeneous function of r with the degree of homogeneity $-D_0$ where $D_0=\ln 2/\ln(1/\gamma)$. D_0 is called self-similarity dimension [5]. Substituting the value of γ in the $3d$ case we obtain $D_0=1/2m$, depending solely on the parameter of the interaction potential.

From the above argument it follows that the number of covering boxes varies as r^{-D_0} with the resolution r, and the number of elements of the object within a sphere of radius R must scale as R^{D_0}. The crucial point to be stressed here is that the above treatment, leading to the self-similarity dimension, considers independently all the elements of the cascade, but neglects the geometrical correlations, and the possible overlapping of different parts of the cascade. That is why for $m<\frac{1}{6}$ the self-similarity dimension D_0 can even exceed the dimension of the embedding space d, and the radius of gyration R_N calculated from the relation $R_N\sim N^{1/D_0}$ underestimates the actual value of R for a given N.

We studied the structure of the vacancy distribution of cascades using MC simulation, so we had random geometrical objects. In this case the fractal dimension D is defined through the scaling behavior of the total number of the vacancies N as a function of the radius of gyration R_N, namely, $N\sim R_N^D$ The radius of gyration is a measure of the linear extension of the cascade, defined as the averaged distance of the vacancy pairs r_{ij} in the cascade,

$$R_N^2=\frac{2}{N(N-1)}\sum_{i<j}^{N} r_{ij}^2. \tag{3}$$

The number of vacancies and the radius of gyration are functions of the bombarding energy. That is why we performed numerical simulations over a wide range of the bombarding energy for each m value to vary the number of vacancies for

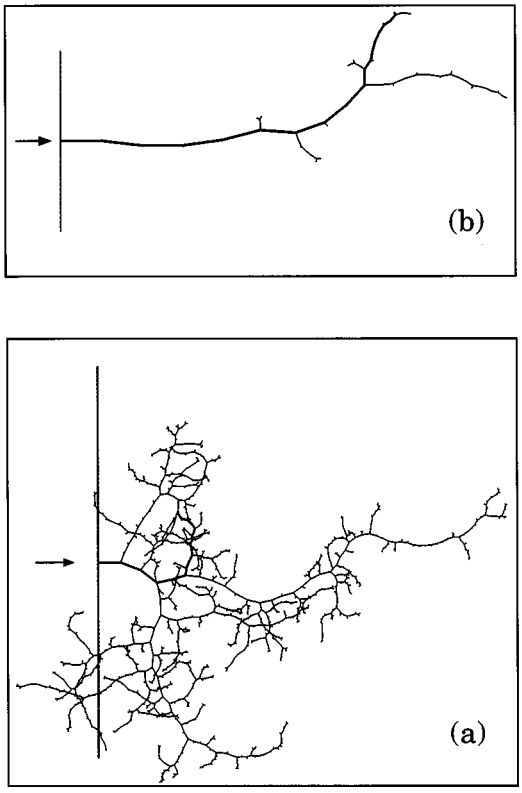

FIG. 2. Simulated cascades in the $2d$ model at two different values of the parameter m, (a) $m=0.5$ and (b) $m=0.85$. The arrow indicates the point where the bombarding particle penetrated the solid, and the fat line shows its path. The solid is supposed to be amorphous and infinite, thus the backscattered particles in (a) cannot leave the solid. For decreasing m the structure of the cascade becomes richer. Since the number of subbranches is increasing, they tend to overlap each other.

the determination of the fractal dimension. The fractal dimension D was extracted from the form

$$N \sim \langle R_N \rangle^D, \tag{4}$$

where the brackets $\langle \cdots \rangle$ denote the average over many cascades containing the same number of vacancies N.

Numerical simulations were performed in $2d$ and $3d$ in a wide range of the parameter m. In $3d$ for the case of the interaction potential Eq. (1) the scattering cross section $d\sigma = CE^{-m}T^{-1-m}dT$ was used for the simulation, where E is the kinetic energy of the moving particle and T is the transferred energy during the scattering process. In $2d$ we constructed a toy model with the scattering cross section $d\sigma = KE^{-m/2}T^{-1-m/2}dT$. In all the simulations particles were stopped when their kinetic energy was smaller than 5 eV. For the $2d$ cascade model one can also construct a substituting deterministic fractal model, but its self-similarity dimension is different from the three dimensional one, namely, $D_0 = 1/m$. Using this toy model in $2d$ we could verify our Flory–de Gennes-type theory, which was originally derived for the three-dimensional case. Figure 2 shows examples of simulated cascades in $2d$. For further details about the MC simulation of collision cascades in the framework of the BCA model, see Refs. [17,18].

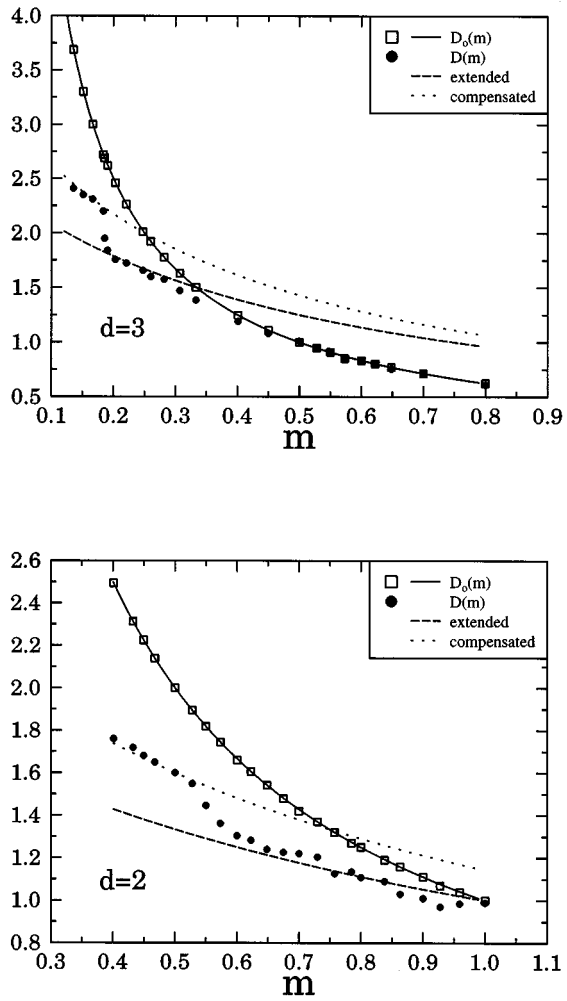

FIG. 3. Comparison of the fractal dimension $D(m)$ extracted from the MC data to the self-similarity dimension $D_0(m)$. The theoretical calculations of the fractal dimension in the extended Eq. (8) and compensated Eq. (9) states are also shown.

The comparison of the fractal dimension $D(m)$ extracted from the numerical data to the self-similarity dimension $D_0(m)$ can be seen in Fig. 3 for $2d$ and $3d$. In $2d$ there is agreement between $D(m)$ and $D_0(m)=1/m$ only in the limit $m \to 1$; for decreasing m the deviation of the two functions is increasing. The curve of $D(m)$ is composed of two distinct smooth parts in the m intervals $0.6<m<1$ and $m<0.52$, with a transient regime in between, $0.52<m<0.6$.

The $3d$ case is more complicated. $D(m)$ is composed of three distinct regimes. For $m>1/3$ there is good agreement between $D(m)$ and $D_0(m)=1/2m$. For $m<1/3$ there is an increasing deviation between the two functions for decreasing m. In the $m<\frac{1}{3}$ region one can distinguish two further smooth parts of $D(m)$ in the intervals of m $0.2<m<1/3$ and $m<0.18$, with a sharp transition in the vicinity of $m=0.19$.

III. FLORY–DE GENNES TYPE MEAN-FIELD APPROACH

If we want to work out a mean-field approach for collision cascades, we face two problems: First, similarly to the case of diffusion-limited aggregation [12–15], there exists no free

energy in the conventional meaning of the term—there exists no attractive or repulsive interaction between the vacancies forming the cascade. Nevertheless, this is not a real problem, since there exists a well-defined probability for the formation of any cascade of any given configuration which can be found by many repetitions of the cascade process, and, so long as the asymptotic $N\to\infty$ properties of a single cascade are the same as this ensemble average, the use of a Flory–de Gennes argument should be valid. The free energy $F(R,N)$, which we estimate, is in fact to within a constant term simply the negative of the logarithm of the total probability $P(R,N)$ for the formation of any cascade of N vacancies with radius of gyration R, or $P(R,N)\sim\exp[-F(R,N)]$.

Furthermore, for a Flory–de Gennes-type argument, the essential properties of the cascade itself are required. Thus at first we have to consider the basic properties of the formation of a collision cascade.

Basically, the cascade is composed of subcascades. The subcascades are generated by the recoiled atoms. If we vary the parameter of the potential m from one toward zero, the probability of displacement will be increased, and the subcascades will contain more and more vacancies. Thus for a certain value of m there will be so many vacancies in the structure that the subcascades tend to overlap each other. Our idea is that the reason for the discrepancy between the measured fractal dimension and the self-similarity dimension is that there are geometrical correlations in the structure due to the overlapping of the subcascades, and this is not taken into account in the derivation of the self-similarity dimension.

The notion of the upper critical dimension used in the study of geometrical structures is analogous to the critical dimension of the thermodynamical systems. The critical dimension $d_c=4$ is the Euclidean dimension above which thermal correlations in a critical system become unimportant, and the critical exponents take their mean-field values. For collision cascades the upper critical dimension d_u is the Euclidean dimension above which the overlapping effect is negligible, and the fractal dimension is equal to the self-similarity dimension $D=D_0$.

The average density of a nonintersecting cascade is $\rho_0\sim R_{N0}^{D_0-d}$. If some parts of the cascade overlap each other, the total number of intersection points would be $R^d\rho_0\rho_0\sim R_{N0}^{2D_0-d}$; this would be the number of particle-particle contacts. It follows that the upper critical dimension is $d_u=2D_0$ for a cascade having a self-similarity dimension D_0. If $d>d_u=2D_0$ the self-intersections are negligible. Now one can explain the deviation of D and D_0 observed in Fig. 3 in $2d$ and $3d$. The self-similarity dimension D_0 depends on m, which is why d_u also has m dependence. In $3d$, while m is greater than $\frac{1}{3}$, the upper critical dimension is smaller than 3, i.e. $d_u<d$. The simulations showed that in this m region $D\sim D_0$, as we expect from the above arguments. In the Family classification scheme this state of random fractals, when geometrical correlations are negligible, is called the ideal state. If $m<\frac{1}{3}$, then $d_u>d$ and the self-intersections become important, resulting in $D<D_0$. In $2d$ we obtain $d_u=2D_0\geqslant d=2$; there is equality solely for $m=1$ (ideal state). Thus the overlap has a dominating role; there is agreement between D and D_0 only in the limiting case of $m=1$, but for $m<1$ we see always deviation.

The Flory–de Gennes approach is based on finding the most probable conformation of an object from an approximate free energy $F(R,N)$. The free energy is a sum of the ''elastic'' and ''repulsive'' terms [11]. The elastic free energy (i.e., the entropic term) tends to make the cluster radius R_N equal to its radius R_{N0} in the ideal state where there are no self-intersections. The elastic free energy is written

$$F_{\rm el}=\frac{R_N^2}{R_{N0}^2}. \tag{5}$$

This term is assumed to be the same for any random structure [11]. The repulsive part of the free energy takes into account the geometrical correlations caused by self-intersections. It is proportional to the number of particle-particle contacts, i.e., $R_N^d\rho\rho$, where $\rho=N/R_N^d$ is the density of the object [11]. Thus for the repulsive part we obtain

$$F_{\rm rep}=A\frac{N^2}{R_N^d}. \tag{6}$$

(This is a mean-field-type approach in the sense that the elements of the fractal are spread over a volume R_N^d, neglecting the possible density fluctuations.) At the beginning let us suppose that A is constant, and independent of N. Minimizing the total free energy F,

$$F=F_{\rm el}+F_{\rm rep}=\frac{R_N^2}{R_{N0}^2}+A\frac{N^2}{R_N^d}, \tag{7}$$

with respect to R_N, keeping R_{N0} and N fixed, and using the definition of the fractal dimension $N\sim R_N^D$, we obtain

$$D=\frac{2+d}{2+(2/D_0)}. \tag{8}$$

This expression of D has two important features. First, it strongly depends on the embedding dimension d and, second, if $d=2D_0$, we obtain $D=D_0$, in agreement with our above upper critical dimension $d_u=2D_0$. If $d>d_u=(2D_0)$ the repulsive part in F is negligible, and the elastic part determines the structure leading to $D=D_0$. In the Family classification scheme this state of random fractals is called an extended state, because this is the most ramified possible conformation of a random fractal in the presence of geometrical correlations. In Eq. (8), D has m dependence through D_0. In Fig. 3 one can see that the predicted curve of the fractal dimension in the extended state Eq. (8) is in good agreement with the measured fractal dimension in $2d$ for $0.6<m$ and in $3d$ for $0.2<m<1/3$.

If we decrease m in the extended state, we reach a point where the multiple overlapping of the subcascades occurs, leading to a more compact shape. It can be simply shown that for the object having self-similarity dimension D_0 the critical dimension of the multiple overlapping $d_u^m=\frac{3}{2}D_0$. If the embedding dimension d is smaller than the critical dimension of the multiple overlapping, the presence of the multiply overlapped regions can increase the fractal dimension D, and we have to modify our argument leading to Eq. (8). Let us suppose that A depends on N as $A\sim N^{-x}$. It can

be interpreted as a kind of screening of the particle-particle ''repulsion,'' which is why, in the Family classification scheme, this state of random fractals is called a compensated state. The value of x can be determined from the requirement that the repulsive part of the free energy should be negligible if $d>d_u^m$. For x we obtain $D_0(2-x)=d_u^m$, and substituting $d_u^m=\frac{3}{2}D_0$ we have $x=0.5$. For the fractal dimension, using the same procedure as above, we obtain

$$D=\frac{2+d}{2-x+(2/D_0)}, \tag{9}$$

which depends on x. The appearance of x in the denominator gives rise to increment of the fractal dimension comparing to the extended state. Figure 3 shows the comparison of the fractal dimension in the compensated state to the MC fractal dimensions. Good agreement is observed in $2d$ for $m<0.52$ and in $3d$ for $m<0.18$. For decreasing m in the compensated state, the fractal dimension increases up to the dimension of the embedding space, resulting in a space-filling compact shape of the cascade.

The overlap of subcascades play an important role in the creation of small amorphous zones in the target. An amorphous zone is formed when either the deposited energy density or the local fractional damage exceeds a critical value. This separates the thermal and displacement spike concepts. An unexpected nonlinear dependence of the damage on the deposited energy was found experimentally; see, e.g., Ref. [16]. The experimental data could be well explained with the assumption of cascade overlap.

At high enough recoil density it becomes possible that the moving particles can collide with each other, and not only with the stationary target atoms. These regions are called thermal spikes, where the majority of atoms are temporarily in motion, giving rise to thermalization. This may occur at the final stage of the cascade evolution. In an actual cascade the parameter m of the effective interaction potential is a function of the kinetic energy of the moving particle; e.g., in the keV energy range $m=\frac{1}{2}$ is a fair approximation, while in the lower eV range $m\leqslant\frac{1}{6}$. Cheng, Nicolet, and Johnson proposed a condition for the thermal spike formation based on the fractal nature of collision cascades. That is, a thermal spike is formed when the self-similarity dimension D_0 of the cascade reaches the dimension of the embedding space d [5]. In the above $2d$ and $3d$ models, this occurs at $m=0.5$ and 0.1666, respectively.

Since the self-similarity dimension $D_0(m)$ and the fractal dimension $D(m)$ of the cascade differ considerably, we have to reconsider the above condition. The density ρ of the displaced atoms N_c with respect to the total number of target atoms N_a in the cascade region is

$$\rho=\frac{N_c}{N_a}\sim R^{D(m)-d}\sim N_c^{[D(m)-d]/D(m)} \tag{10}$$

where $D(m)$ is our MC measured fractal dimension, and R denotes the radius of gyration. It has been shown above that the measured fractal dimensions have a so called transient regime in the vicinity of $m=0.18$ and 0.52 in $3d$ and $2d$, respectively. These regimes are characterized by the fast increase of $D(m)$, which entails that at a fixed N_c value ρ rapidly increases, and the cascade volume is a rapidly decreasing function of m, indicating a kind of collapse of the cascade tree. Thus we can identify these points as the occurrence of high density spikes. Our characteristic m's are very close to those of Ref. [5]. The difference is that the fractal dimension still remains smaller than the embedding dimension, $D\sim2.4$ in $3d$ and $D\sim1.6$ in $2d$.

IV. CONCLUSION AND OUTLOOK

In the present paper we studied the geometrical structure of the vacancy distribution in collision cascades. Based on a Flory–de Gennes-type theory for the fractal dimension, we established an explicit relation of the type $D=D(D_0,d)$. It was shown that the parameter of the interaction potential m plays the role of a control parameter. For decreasing m a transition takes place in the cascade from an open branching structure, through the extended and compensated states toward the space-filling compact shape. The predictions of our formulas are in good agreement with the MC results.

It was reported by several authors in the literature that, due to the change of m during the cascade evolution, an actual collision cascade may be composed of subsets with locally different fractal dimensions (see, e.g., Refs. [1,2,5,7,8]). To analyze structures which consist of a hierarchy of subsets (density fluctuations) with a spectrum of fractal dimensions the (geometrical) multifractality gives a natural framework [19]. Further investigations in this direction are needed.

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