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On the number of contacts of two polymer chains situated on fractal structures

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Abstract. We study the critical behavior of the number of monomer-monomer contacts for two polymers in a good solvent. Polymers are modeled by two self-avoiding walks situated on fractals that belong to the checkerboard (CB) and X family. Each member of a family is labeled by an odd integer b, $3 \leq b \leq \infty$. By applying the exact Renormalization Group (RG) method, we establish the relevant phase diagrams whereby we calculate the contact critical exponents φ (for the CB and X fractals with $b = 5$ and $b = 7$). The critical exponent φ is associated with power law of the number of sites at which the two polymers are touching each other.

PACS. 64.60.Ak Renormalization-group, fractal, and percolation studies of phase transitions – 36.20.Ey Conformation (statistics and dynamics)

1 Introduction

The self-avoiding walk (SAW) is a random walk that must not contain self-intersections. It has been extensively used as a model of a linear polymer chain in a good solvent. Although an isolated chain is difficult to observe experimentally (even at high polymer dilution), numerous studies of the single chain statistics have been upheld as an essential step towards understanding more challenging many-chain systems. A plausible extension of the single polymer concept is the model of two chains in a solvent (good for both chains) [1] whose properties can be also investigated by studying statistics of two SAWs on a lattice [2]. However, the corresponding investigations appears to be difficult if we assume the presence of inter-chain interactions. In this paper we study two chemically different polymers that are situated on the bottom of a shallow container, and which are coupled by a considerable crosslinking interaction. Such a situation can be modelled by two mutually crossing self-avoiding walks, that is, by two SAWs whose paths on a two-dimensional lattice may intersect (cross) each other. Each crossing of the paths corresponds to a contact of two different monomers, and therefore with each crossing we may associate the contact energy ϵ_c. In analogy with the problem of polymer interaction with a penetrable surface [3], we expect to find that with decreasing of temperature the number of crossings M increases so that at the critical temperature T_c it behaves according to the power law

$$M \sim N^{\varphi}, \tag{1}$$

where N is the total number of monomers in the longer chain. Below T_c the number of crossings becomes proportional to N, whereas above T_c it is vanishingly small.

The problem of two chemically different polymers in a good solvent has been extensively studied experimentally [4–6] and theoretically. Various theoretical techniques have been applied, including the random phase approximation [7–9], renormalization group (RG) methods [10–13], field theoretical approach [14] and Monte Carlo simulations [15], to study models of the polymer system in Euclidean lattices. Recently, the problem of two interacting polymer chains has been studied using simultaneously different models and techniques. Thus, a model of two SAWs which are allowed to cross each other was studied by exact enumeration and the Monte Carlo simulations [16]. On the other hand, a system of two SAWs that are mutually avoiding was studied as a diblock copolymer model [17,18]. Finally, the two-SAW model has been used in attacking the denaturation problem of the DNA molecules [19–22].

However, in spite of these numerous different studies of the polymer problem in the case of the Euclidean lattices, the entire physical picture, achieved so far, is of a phenomenological character, and, for example, there is no exact result for the contact critical exponent φ, except for the study of the corresponding two-dimensional diblock copolymer model [17], in which case it was conjectured

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that $\varphi = 9/16$. For this reason, it has been desirable to extend the relevant study to a family of fractal lattices whose members allow, in principle, exact treatment of the problem, and whose characteristics approach (via the so-called fractal-to-Euclidean crossover) properties of a Euclidean lattice. Besides, the study of the polymer problem on fractal lattices has its own practical importance because real containers of the polymer solvent are in many cases porous media that are often fractals, which means that they display self-similar distribution of voids (obstacles) over three to four orders of magnitudes in length scale. The problem described has been attacked, for the Sierpinski gasket (SG) family of fractals, via an exact RG approach [23,24], and by applying the Monte Carlo renormalization group technique [25]. In addition, the problem of two interacting polymer chains, with the interaction parameters that do not allow intersections, has been studied, using an exact RG approach, on a family of the simplex type of fractals [26].

In this paper we exploit the (RG) method to calculate the contact critical exponent φ for the model of two crossing SAWs situated on the CB fractals and, equivalently, for the X fractals. We have obtained φ for the CB (X) fractals, with $b = 5$ and $b = 7$. Details of the requisite RG transformations are explained in Section 2, while the corresponding analysis is performed in Section 3. In Section 4 we present a summary of the obtained results together with an overall discussion within the framework of the current knowledge of the properties of two interpenetrating polymers.

2 Renormalization group transformations

In this section we are going to apply the RG method to study the two crosslinking polymer chains, in a good solvent, situated on the CB (or X) family of fractals. These fractals have been studied in numerous papers, and consequently we shall give here only the necessary brief account of their basic properties. It starts with recalling the fact that each member of the plane CB and X family is labelled by an odd integer $b \geq 3$ and can be obtained as the result of an infinite iterative process of successive ($r \to r+1$) enlarging the fractal structure b times and replacing the smallest parts of the enlarged structure with the generator (initial structure, $r = 1$). The generator of a CB fractal is a square, of size $b \times b$, composed of b rows of unit squares, so that within each row and each column every other of them is removed, whereas in the case of X fractals instead of unit squares we put crosses composed of squares' diagonals (see Fig. 1). Taking into account the self–similar way of the construction of the fractals, one can easily show that the fractal dimension d_f for an arbitrary CB fractal (as well as for X), specified by b, is equal to $\ln[(b^2+1)/2]/\ln b$, so that d_f acquires the Euclidean value 2 when $b \to \infty$. In order to explore effects of crosslinking of two SAWs on the CB (X) fractals, we introduce the two Boltzmann factors $w = e^{-\epsilon_c/T}$ and $t = e^{-\epsilon_t/T}$, where ϵ_c is energy of two monomers in contact (which occurs at a crossing, or touching, site of SAWs), while ϵ_t is the energy associated with two monomers which are nearest neighbours to a crosslinked site and which are visited by different SAWs (see Fig. 2).

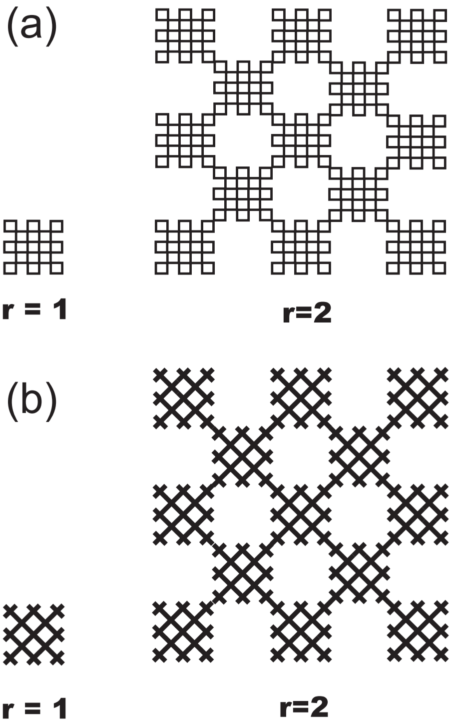

Fig. 1. The first two steps ($r = 1$ and $r = 2$) of the self-similar construction of the CB (a) and X (b) fractals in the case $b = 5$.

If we assign the weight x_1 to a step of the N_1-step SAW and x_2 to a step of the N_2-step SAW, which have M mutual crossings, and there are K pair of sites which are nearest neighbours to crosslinked sites (that are visited by different SAWs), then the corresponding weight of such a configuration is $x_1^{N_1} x_2^{N_2} w^M t^K$. An arbitrary one polymer configuration can be described by using three [27] restricted generating functions, that is, six restricted generating functions for two separated polymers (see Fig. 3). For the r stage fractal structure, these generating functions have the form

$$F_i^{(r)}(x_i) = \sum_{N_i} \mathcal{F}_i{}^{(r)}(N_i) x_i^{N_i}, \qquad i = 1,2, \tag{2}$$

$$G_i^{(r)}(x_i) = \sum_{N_i} \mathcal{G}_i{}^{(r)}(N_i) x_i^{N_i}, \qquad i = 1,2, \tag{3}$$

$$H_i^{(r)}(x_i) = \sum_{N_i} \mathcal{H}_i{}^{(r)}(N_i) x_i^{N_i}, \qquad i = 1,2. \tag{4}$$

To describe all possible configurations of the two crosslinking SAWs we have conceived that we need additional fifteen restricted generating functions (see Fig. 4), which in

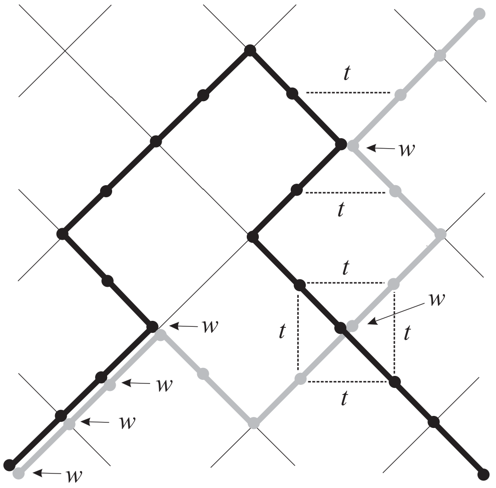

Fig. 2. The $b = 5$ generator of X fractal with segments of two different SAW chains (two different polymers) depicted by black and gray solid lines, while monomers are represented by black and gray bullets. The two SAWs display contacts at the six sites, so that each contact contributes the weight factor w. The dotted lines indicate interaction (characterized by weight factor t) between those monomers which are nearest neighbours to the crosslinked points. Thus, the depicted two-SAW configuration should contribute the weight $x_1^{18} x_2^{14} w^6 t^6$ in the corresponding RG equations (more specifically, in the equation (5) for $i = 2$ and $r = 1$).

terms of the interaction parameters have the form

$$P_i^{(r)}(x_1, x_2, w, t) = \sum_{N_1,N_2,M,K} \mathcal{P}_i{}^{(r)}(N_1, N_2, M, K) \, x_1^{N_1} x_2^{N_2} w^M t^K, \qquad i = 1, 2, 3, \tag{5}$$

$$Q_i^{(r)}(x_1, x_2, w, t) = \sum_{N_1,N_2,M,K} \mathcal{Q}_i{}^{(r)}(N_1, N_2, M, K) \, x_1^{N_1} x_2^{N_2} w^M t^K, \qquad i = 1, 2, 3, 4, \tag{6}$$

$$R_i^{(r)}(x_1, x_2, w, t) = \sum_{N_1,N_2,M,K} \mathcal{R}_i{}^{(r)}(N_1, N_2, M, K) \, x_1^{N_1} x_2^{N_2} w^M t^K, \qquad i = 1, 2, 3, \tag{7}$$

$$S_i^{(r)}(x_1, x_2, w, t) = \sum_{N_1,N_2,M,K} \mathcal{S}_i{}^{(r)}(N_1, N_2, M, K) \, x_1^{N_1} x_2^{N_2} w^M t^K, \qquad i = 1, 2, 3, \tag{8}$$

$$T_i^{(r)}(x_1, x_2, w, t) = \sum_{N_1,N_2,M,K} \mathcal{T}_i{}^{(r)}(N_1, N_2, M, K) \, x_1^{N_1} x_2^{N_2} w^M t^K, \qquad i = 1, 2. \tag{9}$$

Each set of coefficients $(\mathcal{P}_i, \mathcal{Q}_i, \mathcal{R}_i, \mathcal{S}_i, \mathcal{T}_i)$ in the above sums have definite meaning that reflects the corresponding two-polymer configurations (see Fig. 4). In what follows we shall respectively describe each set of coefficients.

$\mathcal{P}_i{}^{(r)}(N_1, N_2, M, K)$ is the number of two-chain configurations, such that each chain is of the F type (see Fig. 3).

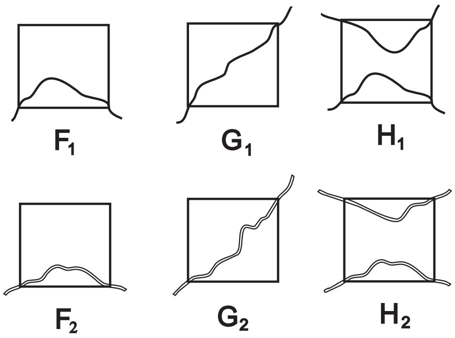

Fig. 3. Schematic representation of the six basic restricted partition functions, at the rth stage fractal structure, needed to obtain all possible configurations of two separated polymer chains (chain 1 is depicted by the solid wiggled line, while the chain 2 is depicted by the wiggled tube).

These chains, with N_1 and N_2 monomers, have M mutual crossings, and posses K pair of sites which are nearest neighbours to crosslinked sites, that belong to different chains (this meaning of M and K stays valid for the rest four sets of coefficients).

$\mathcal{Q}_i{}^{(r)}(N_1, N_2, M, K)$ is the number of two-chain configurations, such that each chain is either of F or of G type, but excluding situations when both are of F type.

$\mathcal{R}_i{}^{(r)}(N_1, N_2, M, K)$ (and similarly $\mathcal{S}_i{}^{(r)}(N_1,\ N_2,\ M,\ K)$) is the number of two-chain configurations, such that only one chain is of the H type, while the other chain must be of the F or G type (see Fig. 3).

Finally, the coefficients $\mathcal{T}_i{}^{(r)}(N_1, N_2, M, K)$ is the number of two-chain configurations, such that bout chains are of the H type.

These generating functions (depicted in Figs. 3 and 4) appears to be parameters in the renormalization group (RG) approach. It can be verified that in the $b = 3$ case the system under study would be forced to stay in a finite piece of the underlying fractal lattice [27,28], while for any $b \geq 5$ the RG equations have the form

$$F_i^{(r+1)} = \sum_{j_1,j_2,j_3} f_i(j_1, j_2, j_3) F_i^{j_1} G_i^{j_2} H_i^{j_3}, \qquad i = 1, 2, \tag{10}$$

$$G_i^{(r+1)} = \sum_{j_1,j_2,j_3} g_i(j_1, j_2, j_3) F_i^{j_1} G_i^{j_2} H_i^{j_3}, \qquad i = 1, 2, \tag{11}$$

$$H_i^{(r+1)} = \sum_{j_1,j_2,j_3} h_i(j_1, j_2, j_3) F_i^{j_1} G_i^{j_2} H_i^{j_3}, \qquad i = 1, 2, \tag{12}$$

$$P_i^{(r+1)} = \sum_{j_1,\ldots,j_{21}} p_i(j_1, \ldots, j_{21}) F_1^{j_1} G_1^{j_2} H_1^{j_3} F_2^{j_4} G_2^{j_5} H_2^{j_6} P_1^{j_7} P_2^{j_8} P_3^{j_9} Q_1^{j_{10}} Q_2^{j_{11}} Q_3^{j_{12}} Q_4^{j_{13}} R_1^{j_{14}} R_2^{j_{15}} R_3^{j_{16}} S_1^{j_{17}} S_2^{j_{18}} S_3^{j_{19}} T_1^{j_{20}} T_2^{j_{21}}, \qquad i = 1, 2, 3, \tag{13}$$

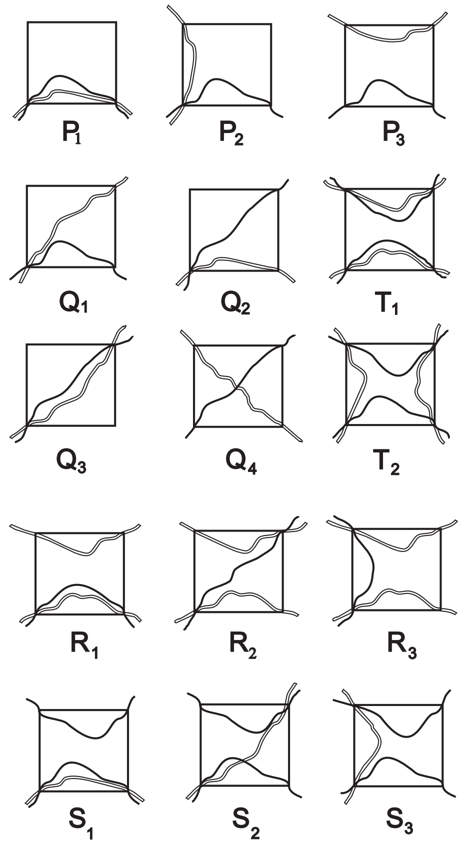

Fig. 4. Schematic representation of the fifteen restricted generating functions used in describing all possible two-polymer configurations within the rth stage CB (or X) fractal structure. Thus, for example, P_1 represents the polymers' paths that start at the lower left vertex and exit at the lower right vertex. The interior details of the rth order fractal structure are not shown (they are manifested by the wiggles of the paths).

$$Q_i^{(r+1)} = \sum_{j_1,\ldots,j_{21}} q_i(j_1,\ldots,j_{21}) F_1^{j_1} G_1^{j_2} H_1^{j_3} F_2^{j_4} G_2^{j_5} H_2^{j_6} P_1^{j_7} P_2^{j_8} P_3^{j_9} Q_1^{j_{10}} Q_2^{j_{11}} Q_3^{j_{12}} Q_4^{j_{13}} R_1^{j_{14}} R_2^{j_{15}} R_3^{j_{16}} S_1^{j_{17}} S_2^{j_{18}} S_3^{j_{19}} T_1^{j_{20}} T_2^{j_{21}}, \quad i = 1,2,3,4, \quad (14)$$

$$R_i^{(r+1)} = \sum_{j_1,\ldots,j_{21}} r_i(j_1,\ldots,j_{21}) F_1^{j_1} G_1^{j_2} H_1^{j_3} F_2^{j_4} G_2^{j_5} H_2^{j_6} P_1^{j_7} P_2^{j_8} P_3^{j_9} Q_1^{j_{10}} Q_2^{j_{11}} Q_3^{j_{12}} Q_4^{j_{13}} R_1^{j_{14}} R_2^{j_{15}} R_3^{j_{16}} S_1^{j_{17}} S_2^{j_{18}} S_3^{j_{19}} T_1^{j_{20}} T_2^{j_{21}}, \quad i = 1,2,3, \quad (15)$$

$$S_i^{(r+1)} = \sum_{j_1,\ldots,j_{21}} s_i(j_1,\ldots,j_{21}) F_1^{j_1} G_1^{j_2} H_1^{j_3} F_2^{j_4} G_2^{j_5} H_2^{j_6} P_1^{j_7} P_2^{j_8} P_3^{j_9} Q_1^{j_{10}} Q_2^{j_{11}} Q_3^{j_{12}} Q_4^{j_{13}} R_1^{j_{14}} R_2^{j_{15}} R_3^{j_{16}} S_1^{j_{17}} S_2^{j_{18}} S_3^{j_{19}} T_1^{j_{20}} T_2^{j_{21}}, \quad i = 1,2,3, \quad (16)$$

$$T_i^{(r+1)} = \sum_{j_1,\ldots,j_{21}} t_i(j_1,\ldots,j_{21}) F_1^{j_1} G_1^{j_2} H_1^{j_3} F_2^{j_4} G_2^{j_5} H_2^{j_6} P_1^{j_7} P_2^{j_8} P_3^{j_9} Q_1^{j_{10}} Q_2^{j_{11}} Q_3^{j_{12}} Q_4^{j_{13}} R_1^{j_{14}} R_2^{j_{15}} R_3^{j_{16}} S_1^{j_{17}} S_2^{j_{18}} S_3^{j_{19}} T_1^{j_{20}} T_2^{j_{21}}, \quad i = 1,2, \quad (17)$$

where we have omitted the superscript (r) on the right-hand side of the above relations. The self-similarity of the fractals implies that numbers $\{f_i(j_1,j_2,j_3),\ g_i(j_1,j_2,j_3),\ h_i(j_1,j_2,j_3)\}$ which describe configurations of a polymer chain, and that numbers $\{p_i(j_1,\ldots,j_{21}),\ q_i(j_1,\ldots,j_{21}),\ r_i(j_1,\ldots,j_{21}),\ s_i(j_1,\ldots,j_{21}),\ t_i(j_1,\ldots,j_{21})\}$ of the corresponding two-chain configurations do not depend on r. Starting with the initial conditions

$$\begin{aligned}
F_i^{(0)}(x_i) = G_i^{(0)}(x_i) = x_i^2, H_i^{(0)} = 0, &\qquad i = 1,2;\\
P_1^{(0)}(x_1,x_2,w,t) &= x_1^2 x_2^2 w^2,\\
P_2^{(0)}(x_1,x_2,w,t) &= x_1^2 x_2^2 w^{3/2},\\
P_3^{(0)}(x_1,x_2,w,t) &= x_1^2 x_2^2 w t^2,\\
Q_1^{(0)}(x_1,x_2,w,t) = Q_2^{(0)}(x_1,x_2,w,t) &= x_1^2 x_2^2 w^{3/2} t,\\
Q_3^{(0)}(x_1,x_2,w) &= x_1^2 x_2^2 w^2,\\
Q_4^{(0)}(x_1,x_2,w,t) &= x_1^2 x_2^2 w t^4,\\
S_i^{(0)} = R_i^{(0)} &= 0, \qquad i = 1,2,3;\\
T_i^{(0)} &= 0, \qquad i = 1,2, \qquad (18)
\end{aligned}$$

(which for the X fractals correspond to the crosses comprised of squares' diagonals) one can iterate the RG relations (10–17) for various values of interactions w and t, and explore the resulting phase diagram.

3 Analysis of the RG equations

To solve exactly the problem of two mutually crossing SAWs, for arbitrary member (arbitrary $b \geq 3$) of the X (CB) family, it is necessary to find all coefficients that appear in the RG equations (10–17). The $b = 3$ case would not reveal physically interesting results (as it was already noted, the system under study would be forced to stay in a finite piece of the underlying fractal lattice). On the other hand, for the $b = 5, 7$ and $b = 9$ fractals only RG equations (10, 11) and (12), that correspond to the one polymer case, have been studied [27]. In this paper we undertake a thorough analysis of the $b = 5$ and $b = 7$ RG transformations for two crosslinked polymers, which requires analysis of an additional set of equations (13–17). Thus, the complete set of the RG transformations is (10–17), and it should be analyzed together with the corresponding initial conditions (18).

On the physical grounds that are plausible for the problem under study (see, for example [25]), one can expect that the RG transformations should have three relevant fixed points of the general type

$$(F_1^*, G_1^*, H_1^*, F_2^*, G_2^*, H_2^*, P_1^*, P_2^*, P_3^*, Q_1^*, Q_2^*, Q_3^*, Q_4^*, R_1^*, R_2^*, R_3^*, S_1^*, S_2^*, S_3^*, T_1^*, T_2^*). \quad (19)$$

The first fixed point

$$(F^*, G^*, H^*, F^*, G^*, H^*, 0, 0, H^*, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0), \quad (20)$$

with $P_1^* = P_2^* = 0$, $P_3^* = H^*$, $Q_i^* = 0$ $(i = 1, 2, 3, 4)$, $R_i^* = S_i^* = 0$ $(i = 1, 2, 3)$ and $T_i^* = 0$ $(i = 1, 2)$, due to the meaning of these quantities (see Figs. 3 and 4), describes segregated phase of two chain polymers that should be expected in the high temperature region. The second fixed point

$$\begin{aligned}(F^*, G^*, H^*, F^*, G^*, H^*, (F^*)^2, (F^*)^2, (F^*)^2,\\ F^*G^*, F^*G^*, (G^*)^2, (G^*)^2, F^*H^*, G^*H^*, F^*H^*,\\ F^*H^*, G^*H^*, F^*H^*, (H^*)^2, (H^*)^2),\end{aligned} \qquad (21)$$

with $P_i^* = (F^*)^2$ $(i = 1, 2, 3)$, $Q_1^* = Q_2^* = F^*G^*$, $Q_3^* = Q_4^* = (G^*)^2$, $S_1^* = S_3^* = R_1^* = R_3^* = F^*H^*$, $S_2^* = R_2^* = G^*H^*$ and $T_1^* = T_2^* = (H^*)^2$, which appears to be a tricritical point, describes the state of the two-polymer system that occurs at the critical temperature $T = T_c$ when segregated and entangled polymer phases become identical. Finally, the third fixed point

$$(0, 0, 0, 0, 0, 0, F^*, 0, 0, 0, 0, G^*, 0, 0, 0, 0, 0, 0, 0, H^*, 0). \qquad (22)$$

with $P_1^* = F^*$, $Q_3^* = G^*$ and $T_1^* = H^*$, describes the polymer entangled state, which should emerge at low temperatures.

In what follows we focus our attention on the tricritical fixed point (21) to calculate the contact critical exponent φ. It should be observed that, for each b, equations (10–12), have only one nontrivial fixed point value $F_1^* = F_2^* = F^*$, $G_1^* = G_2^* = G^*$ and $H_1^* = H_2^* = H^*$ [27], which thereby completely determines the tricritical fixed point. Calculation of the contact critical exponent φ starts with solving the eigenvalue problem of the RG equations (10–12), linearized at the tricritical fixed point. Here it should be noticed that the RG equations (10–12), for $i = 1$ and $i = 2$, have the identical structure, and, in addition, they are not coupled with the other 15 RG equations (13–17), which implies that the eigenvalue problem can be separated into two parts. The first part of the eigenvalue problem, related to the equations (10–12) (for $i = 1$, or $i = 2$) gives the eigenvalue λ_ν of the end–to–end distance critical exponent $\nu = \ln b / \ln \lambda_\nu$. The second part of the eigenvalue problem reduces to solving the equation

$$\det \left| \left(\frac{\partial X_i'}{\partial X_j} \right)^* - \lambda\, \delta_{i,j} \right| = 0, \qquad (23)$$

where X_i are elements of the set $\{P_1, P_2, P_3, Q_1, Q_2, Q_3, Q_4, R_1, R_2, R_3, S_1, S_2, S_3, T_1, T_2\}$, and the asterisk means that the derivatives should be taken at the tricritical fixed point. Also, we have used the prime symbol as a superscript for the $(r + 1)$–th restricted partition functions and no indices for the rth order partition functions. The largest eigenvalue λ_φ of above equation determine the contact critical exponent through the formula

$$\varphi = \frac{\ln \lambda_\varphi}{\ln \lambda_\nu}. \qquad (24)$$

Hence, in an exact RG evaluation of φ one needs to calculate partial derivatives of sums (10–17), and accordingly one should find the coefficients $f_i(j_1, j_2, j_3)$, $g_i(j_1, j_2, j_3)$, $h_i(j_1, j_2, j_3)$, $p_i(j_1, \ldots, j_{21})$, $q_i(j_1, \ldots, j_{21})$, $r_i(j_1, \ldots, j_{21})$, $s_i(j_1, \ldots, j_{21})$, and $t_i(j_1, \ldots, j_{21})$, by an exact enumeration of all possible SAWs for each particular b. We have enumerated the needed coefficients by using computer facilities of a personal computer with the Intel Pentium 4 CPU. The corresponding enumerations are very cumbersome because of the very large number of possible configurations. For instance, the coefficient $p_2(j_1, \ldots, j_{21})$, in the $b = 5$ case, has 282 nonzero values which spring from 324 different polymer configurations of the P_2 type (see Fig. 4). For the sake of comparison, we quote here that the same coefficient, in the case $b = 7$, has 90598 nonzero values which is related to the 292 677 different polymer configurations. Therefore, it is impossible to quote these coefficients (the authors of this paper are willing to provide, upon a request, all these data by electronic means).

We have first analyzed the complex system of the RG equations for $b = 5$, in order to locate the relevant fixed points. After an extensive numerical analysis we have found three fixed points. The first one describes critical properties of the segregate phase of the two-chain polymer system. Its coordinates, written in the way accepted in (20), are specified by $F^* = 0.663711$, $G^* = 0.724640$ and $H^* = 0.100029$. The specified values stay valid for the tricritical fixed point (21), and for the third one (22) that describe the entangled polymer phase.

To learn the physical behaviour of the system under study we have repeatedly performed mapping of the interaction parameters using the established RG transformations, together with the concomitant initial conditions (18). The obtained phase diagram is depicted in Figure 5, in which one may follow the critical fugacity x_c curve for the X fractal as a function of the parameter w for various values of t. When the RG transformations (10–17) are iterated by starting at the horizontal part of the curves $x_c = x_c^*$ (at small values of w) the fixed point (20), which describes the segregate phase of the two chain polymer system, is reached. On the other hand, if the iterations start at the part of the critical fugacity curve $x_c = x_c(w)$ that appears beyond the point $(w_c^*(t_i), x_c^*)$ the polymer entangled state fixed point (22) is achieved. Finally, when the RG iteration starts at the points $(w_c^*(t), x_c^*)$, where the curves which correspond to the segregate phase join with the curves of the entangled polymer phases, it leads to the tricritical fixed point (21). In addition to the presented graphic, we give here our finding for the specific value of the contact critical exponent φ. In the $b = 5$ case, we have found $\lambda_\varphi = 4.529696$, which together with the previously found [27] value $\lambda_\nu = 6.607689$, through formula (24), gives $\varphi = 0.800036$. Before passing further, we find sensible to note that $\lambda_\nu = 6.607689$ brings about $\nu = 0.85235$.

In the case $b = 7$ fractal we can expect to find the same type of the phase diagram as in the case $b = 5$ (see Fig. 5). To obtain the same set of data discussed above (for $b = 5$), we need to perform a similar kind of analysis of the corresponding RG transformations. However, in this case one encounters a specific computational problem, that is, we have been able to calculate all the

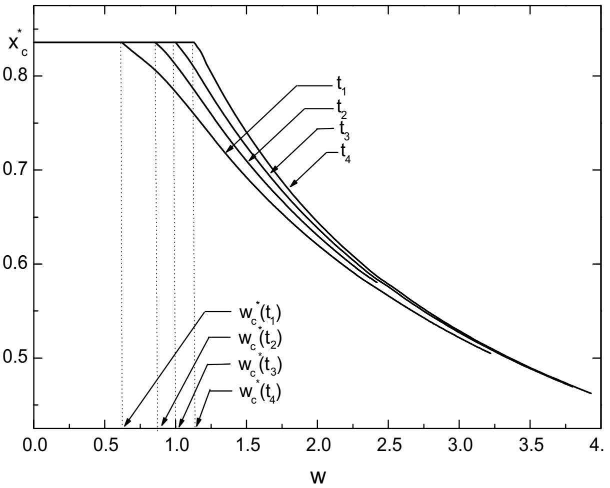

Fig. 5. The critical fugacity x_c curve for the X fractal, with the base $b = 5$, as a function of the parameter w for various values of t, $(t_1 > t_2 > t_3 = 1 > t_4)$. The RG transformations (10–17) iterated by starting at the horizontal part of the curves $x_c = x_c^*$ lead to the fixed point (20), which describes the segregate phase of the two chain polymer system. On the other hand, if the iterations start at the part of the critical fugacity curve $x_c = x_c(w)$ that appears beyond the point $(w_c^*(t_i), x_c^*)$, $i = 1, 2, 3$, and 4, it leads to the polymer entangled state fixed point (22). Finally, when the RG iteration starts at the point $(w_c^*(t_i), x_c^*)$ it reaches the tricritical fixed point (21).

requisite coefficients of the RG transformations (10–17), but it was impossible to store all of them in the memory of the available computer system. Fortunately, we have found means to surmount this problem by observing that neglecting the partition functions of the H_i type (see Fig. 3), as well as those functions $(S_i, R_i, T_i$, see Fig. 4) that are comprised of H_i, does not cause significant errors in the results for the critical exponents. To corroborate this approach, we analyzed in this manner the $b = 5$ case, where we have available exact results. Thus, for $b = 5$, we obtained the following coordinates for the relevant fixed points $F^* = 0.659119$, $G^* = 0.737227$ and $H^* \equiv 0$ which brings about $\nu = 0.86098$ and $\varphi = 0.797108$. Comparing the latter two approximate values with the exact findings $\nu = 0.85235$ and $\varphi = 0.800036$, one can observe the following deviations $\delta_\nu = 1.02\%$ and $\delta_\varphi = 0.36\%$. Thus, one may conclude that the suggested approximate approach $(H^* \equiv 0)$ could not cause significant errors. Moreover, we may expect that for larger b deviations gradually decrease [25].

Accepting in the case $b = 7$ the method suggested in the foregoing paragraph, we get the following values of coordinates for the relevant fixed points $F^* = 0.569527$, $G^* = 0.627881$ and $H^* \equiv 0$, which provides new results within the scope of the studied problem, that is, $\nu = 0.820009$ and $\varphi = 0.670485$. Comparing the obtained value for ν with the exact [27] value $\nu = 0.81502$ we discover that the relevant deviation $\delta_\nu = 0.63\%$ is almost two times smaller than in the case when the same method was applied for $b = 5$. On these grounds, we may expect that the obtained value for the critical exponent φ should not deviate from the exact value more that 0.23%.

4 Summary and discussion

In this paper we have studied the statistical properties of two chemically different polymers that display recognizable monomer–monomer crosslinking interaction. Such a situation can be modelled by two mutually crossing self-avoiding walks (SAWs) on a appropriate lattice. In order to explore effects of crosslinking of the two SAWs on the CB (X) fractals, we have introduced the two weighting factors $w = e^{-\epsilon_c/T}$ and $t = e^{-\epsilon_t/T}$, where ϵ_c is energy of two monomers in contact (which occurs at a crossing site of SAWs), while ϵ_t is the energy associated with two monomers which are nearest neighbours of the crosslinked site and which belong to different polymers. To obtain specific results for the problem under study, we have applied the exact RG method in the case of the CB fractals and X fractals, and for their specific cases labelled by $b = 5$ and $b = 7$ (the cases with $b > 7$ are not amenable to the exact approach).

In both cases ($b = 5$ and $b = 7$) we have found the phase diagrams defined in the planes of the interaction parameters x and w, for various values of t. We have calculated the critical curves whose two consecutive segments (which determine, depending on the value of w, two different phases, segregate and entangled) meet at the the tricritical point that provides possibility of calculating the contact critical exponent φ. In accordance with presented RG outline, we have found $\varphi = 0.800036$, for $b = 5$, and $\varphi = 0.670485$, for $b = 7$. The difference between the two values reflects the different energies that would be needed to uncouple polymers which have been crosslinked on the two different CB lattices under study (the cases $b = 5$ and $b = 7$). On the other hand, the difference in the values of φ should have been expected because of the difference in the fractal dimensions $(d_f^{CB}(b = 7) > d_f^{CB}(b = 5)$; $d_f^{CB}(b = 7) = 1.65417$ and $d_f^{CB}(b = 5) = 1.59369)$, which causes less possibility for two polymers to come across each other on the $b = 7$ lattice than on the $b = 5$ lattice. Comparing our presented findings with the value $\varphi = 0.516 \pm 0.005$ [16] calculated for the $2d$ Euclidean case, we observe that the latter is smaller than the corresponding values pertinent to the fractal lattices.

The next assessment of our results can be comparison with available results obtained for the same problem analyzed on fractals that have similar topological properties. Unfortunately, presently there is only one case that can be used for such a comparison. We find that the results obtained for the Sierpinski gasket (SG) fractals [23,24] may serve the purpose so as to compare our results with the results for those SG fractals which have approximately the same fractal dimensions as those studied in this work. Consequently, we should compare findings for the $b = 5$ and $b = 7$ CB fractals with the $b = 2$ and $b = 4$ SG fractals, respectively. We find the following inequalities $\varphi_{CB}(5) = 0.800036 > \varphi_{SG}(2) = 0.7491$

and $\varphi_{CB}(7) = 0.670485 < \varphi_{SG}(4) = 0.7117$. Therefore we may put forward the conclusion that the fractal dimension is not the crucial parameter which determines the contact critical exponent φ.

To make comparison of our findings with the existing results, we inspect the phenomenological formula $\varphi_{ph} = 2 - \nu d_f$ [16,24] for $b = 5$ and $b = 7$. The predictions that follow from the preceding formula, $\varphi_{ph}(b = 5) = 0.64162$ and $\varphi_{ph}(b = 7) = 0.65181$, deviate from our exact results 19.8% and 2.78%, respectively. It appears that one can conclude that the deviation of phenomenological prediction from the exact results becomes smaller for the larger scaling parameter b. This observation may be an inspiration for the attempt to find more exact results, or to extend our approach by some reliable approximate means. Within our knowledge of the field, we may expect that the Monte Carlo renormalization group approach may be the most effective choice for the further study of the problem.

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