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# Investigation of the number of contacts of two cross-linked polymer chains on the family of three-dimensional fractal structures

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## Monte Carlo renormalization group approach

3D fractals may serve as a better description of real systems (porous media, for instance).

The two-polymer system is modelled by two SAWs which are allowed to cross each other.

Contact critical exponent φ of two polymer chains describes the number of the two chains contacts.

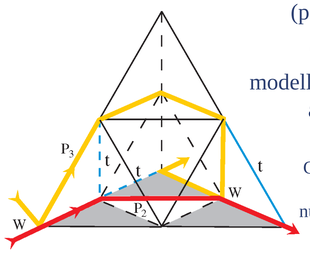


**Figure 1.** The structure of the three-dimensional SG fractal, for b = 2, at the first stage of construction, with an example of the bulk polymer chain (P3) depicted by a yellow line and the surface adsorbed polymer chain (P2) depicted by a red line. The shaded area represents the adsorbing surface (the two-dimensional SG fractal). The two polymers are cross-linked at the two cites, so that each contact contributes the weight factors *w*. The blue bonds, marked 't', describe the interactions between those monomers which are nearest neighbours to the cross-linked points.

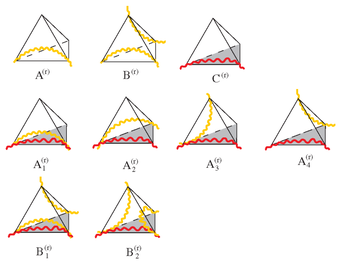


**Figure 2.** Schematic representation of the nine restricted generating functions used in the description of all possible two-SAW configurations, within the *r*th stage of the 3D SG fractal structure. Thus, for example, the $A_1^{(r)}$ represents the configuration when the two polymers (3D SG floating and 2D SG adsorbed) pass through the same vertices of a particular *r*th stage of the fractal lattice. The interior details of the *r*th-stage fractal structure, as well as details of the chains, are not shown (for the chains, they are manifested by the wiggles of the SAW paths).

$$A^{(r+1)} = \sum_{N_A,N_B} a(N_A,N_B)\, A^{N_A} B^{N_B},$$

$$B^{(r+1)} = \sum_{N_A,N_B} b(N_A,N_B)\, A^{N_A} B^{N_B},$$

$$C^{(r+1)} = \sum_{N_C} c(N_C)\, C^{N_C},$$

$$A_i^{(r+1)} = \sum_{\mathcal{N}} a_i(\mathcal{N})\, A^{N_A} B^{N_B} C^{N_C} \prod_{j=1}^{4} A_j^{N_{A_j}} \prod_{k=1}^{2} B_k^{N_{B_k}}, \qquad i = 1,2,3,4,$$

$$B_i^{(r+1)} = \sum_{\mathcal{N}} b_i(\mathcal{N})\, A^{N_A} B^{N_B} C^{N_C} \prod_{j=1}^{4} A_j^{N_{A_j}} \prod_{k=1}^{2} B_k^{N_{B_k}}, \qquad i = 1,2,$$

The above set of relations can be considered as the RG equations for the problem under study, with the initial conditions $A^{(0)} = x_3$, $B^{(0)} = x_3^2$, $C^{(0)} = x_2$, $A_1^{(0)} = x_3x_2w^2$, $A_2^{(0)} = A_3^{(0)} = x_3x_2wt$, $A_4^{(0)} = x_3x_2$ and $B_1^{(0)} = B_2^{(0)} = x_3^2x_2w^2$

Keywords: classical Monte Carlo simulations, critical exponents and amplitudes (theory), renormalization group, polymers

## Results and discussion

Calculation of a long sequence of contact critical exponents values, for a sequence of 3D SG fractals, for $2 \le b \le 40$

The main goal is the MCRG evaluation of $\varphi_{32}$, for various values of *b*. In the case *b* = 2, the exact value was calculated.

$$\varphi_{32}(b=2) = \ln 1.7475 / \ln 2.7965 = 0.5428$$

$$\varphi_{32} = \frac{\ln \lambda_{\varphi_{32}}}{\ln \lambda_{\nu_3}}.$$

Critical exponent $\varphi_{32}$ - the first polymer is a floating 3D SG chain, while the other is a 2D SG adsorbed chain

**Table 1.** The MCRG ($2 \le b \le 40$) results obtained in this work for the contact critical exponents $\varphi_{32}$ for the 3D SG family of fractals.

| *b* | $A^*$ | $B^*$ | $C^*$ | $\varphi_{32}$ |
|---|---|---|---|---|
| 2 | $0.4311 \pm 0.0009$ | $0.0505 \pm 0.0023$ | $0.618\,25 \pm 0.000\,61$ | $0.5440 \pm 0.0056$ |
| 3 | $0.3421 \pm 0.0004$ | $0.0245 \pm 0.0015$ | $0.551\,37 \pm 0.000\,44$ | $0.4969 \pm 0.0024$ |
| 4 | $0.2898 \pm 0.0004$ | $0.0122 \pm 0.0020$ | $0.506\,58 \pm 0.000\,34$ | $0.4658 \pm 0.0006$ |
| 5 | $0.2560 \pm 0.0004$ | $0.0067 \pm 0.0019$ | $0.474\,55 \pm 0.000\,28$ | $0.4451 \pm 0.0012$ |
| 6 | $0.2319 \pm 0.0003$ | $0.0038 \pm 0.0012$ | $0.450\,91 \pm 0.000\,24$ | $0.4250 \pm 0.0004$ |
| 7 | $0.2148 \pm 0.0003$ | $0.0020 \pm 0.0018$ | $0.432\,40 \pm 0.000\,21$ | $0.4092 \pm 0.0008$ |
| 8 | $0.2016 \pm 0.0003$ | $0.0012 \pm 0.0026$ | $0.417\,80 \pm 0.000\,19$ | $0.3963 \pm 0.0006$ |
| 9 | $0.1912 \pm 0.0004$ | $0.0007 \pm 0.0008$ | $0.405\,74 \pm 0.000\,17$ | $0.3841 \pm 0.0007$ |
| 10 | $0.1829 \pm 0.0003$ | $0.0005 \pm 0.0023$ | $0.395\,86 \pm 0.000\,07$ | $0.3714 \pm 0.0005$ |
| 12 | $0.1703 \pm 0.0004$ | $0.0001 \pm 0.0035$ | $0.380\,37 \pm 0.000\,13$ | $0.3514 \pm 0.0004$ |
| 15 | $0.1581 \pm 0.0001$ | — | $0.363\,96 \pm 0.000\,11$ | $0.3226 \pm 0.0003$ |
| 17 | $0.1526 \pm 0.0001$ | — | $0.355\,93 \pm 0.000\,08$ | $0.3126 \pm 0.0003$ |
| 20 | $0.1462 \pm 0.0001$ | — | $0.346\,81 \pm 0.000\,06$ | $0.2956 \pm 0.0003$ |
| 25 | $0.1399 \pm 0.0001$ | — | $0.336\,02 \pm 0.000\,08$ | $0.2677 \pm 0.0003$ |
| 30 | $0.1353 \pm 0.0001$ | — | $0.328\,76 \pm 0.000\,07$ | $0.2573 \pm 0.0002$ |
| 35 | $0.1327 \pm 0.0001$ | — | $0.323\,50 \pm 0.000\,08$ | $0.2183 \pm 0.0003$ |
| 40 | $0.1305 \pm 0.0001$ | — | $0.319\,36 \pm 0.000\,06$ | $0.2016 \pm 0.0003$ |

RG evaluation of $\varphi_{32}$, only for small b
MCRG method for large b

for *b* = 2 fractal (0.5440±0.0056 versus 0.5428) MCRG result deviates by 0.22% from the exact RG result

We find the following phenomenological formula for the contact critical exponent

$$\varphi_{32}^{CA} = \left(1 + \frac{\nu_3}{\nu_2}\right) - \nu_3 d_f^{3D}$$

## Results and discussion

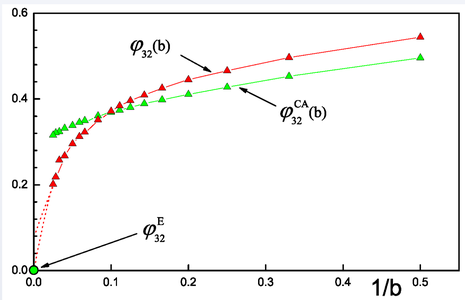


**Figure 3.** Results obtained in this work for the contact critical exponent $\varphi_{32}$ for the two-polymer system, when the first polymer is a floating 3D SG chain, while the other is a 2D SG adsorbed chain. The red triangles represent the MCRG values, while green triangles correspond to the CA values
The green circle depicts the three-dimensional Euclidean value $\varphi_{32}^{E} \approx 0$. The thin solid lines (red and green) represent a simple interpolation of data, while the red dotted lines show the two possible scenarios for the fractal-to-Euclidean behaviour of $\varphi_{32}$, and serve as guides to the eye. The error bars, for the MCRG data, are not depicted in the figure, since in all cases they lie within the corresponding symbols (red triangles).

The critical exponent $\varphi_{33}$ which describes the number of polymer–polymer contacts, when both polymers are floating chains in the 3D SG fractal container (both polymers are of the type P3), and $\varphi_{22}$ when both polymers are adsorbed by the 2D SG surface (both of the type P2). These are the corresponding phenomenological formulae:

$$\varphi_{33}^{CA} = 2 - \nu_3 d_f^{3D}$$

$$\varphi_{22}^{CA} = 2 - \nu_2 d_f^{2D}$$

**Table 2.** Numerical values for the contact critical exponents $\varphi_{32}$, $\varphi_{33}$ and $\varphi_{22}$ evaluated from the proposed phenomenological formulae (based on the CA arguments).

| *b* | $\nu_3$ | $\nu_2$ | $\varphi_{32}^{CA}$ | $\varphi_{33}^{CA}$ | $\varphi_{22}^{CA}$ |
|---|---|---|---|---|---|
| 2 | 0.6742 | 0.7985 | 0.4959 | 0.6516 | 0.7344 |
| 3 | 0.6543 | 0.7937 | 0.4530 | 0.6287 | 0.7055 |
| 4 | 0.6414 | 0.7882 | 0.4277 | 0.6140 | 0.6908 |
| 5 | 0.6315 | 0.7840 | 0.4105 | 0.6050 | 0.6808 |
| 6 | 0.6239 | 0.7801 | 0.3981 | 0.5984 | 0.6745 |
| 7 | 0.6169 | 0.7773 | 0.3890 | 0.5953 | 0.6689 |
| 8 | 0.6130 | 0.7742 | 0.3805 | 0.5887 | 0.6658 |
| 9 | 0.6087 | 0.7722 | 0.3738 | 0.5855 | 0.6622 |
| 10 | 0.6048 | 0.7698 | 0.3690 | 0.5833 | 0.6603 |
| 12 | 0.5987 | 0.7659 | 0.3608 | 0.5792 | 0.6571 |
| 15 | 0.5933 | 0.7620 | 0.3497 | 0.5711 | 0.6529 |
| 17 | 0.5899 | 0.7590 | 0.3455 | 0.5683 | 0.6523 |
| 20 | 0.5869 | 0.7560 | 0.3384 | 0.5621 | 0.6506 |
| 25 | 0.5817 | 0.7516 | 0.3317 | 0.5577 | 0.6495 |
| 30 | 0.5795 | 0.7481 | 0.3249 | 0.5502 | 0.6491 |
| 35 | 0.5759 | 0.7457 | 0.3212 | 0.5490 | 0.6480 |
| 40 | 0.5755 | 0.7434 | 0.3158 | 0.5416 | 0.6479 |

$\varphi_{32} < \varphi_{33} < \varphi_{22}$

The possible behaviour of the contact critical exponents in the fractal-to-Euclidean crossover region: in the limit $b \to \infty$

Euclidean values computed:

$$\varphi_{32}^{E} \approx 0,\ \varphi_{33}^{E} \approx 1/5 \text{ and } \varphi_{22}^{E} = 1/2.$$

## Summary

In this paper we have studied two interacting linear polymer chains, modelled by two mutually crossing self-avoiding walk (SAWs), situated on fractal structures represented by the three-dimensional (3D) Sierpinski gasket (SG) family of fractals. The assumption was set that the first polymer (P3) is a floating chain in the bulk of the 3D SG fractal, while the second polymer chain (P2) is adsorbed on one of the four boundaries of the 3D SG fractal, which appears to be a 2D SG fractal. Specifically, we have calculated the critical exponent $\varphi_{32}$, associated with the number of monomer–monomer contacts between polymers P3 and P2. By applying the renormalization group (RG) method, we have calculated the exact value of the critical exponent $\varphi_{32}$, for the first member b = 2 of the 3D SG fractal family. The specific accomplishment in the course of this work is the calculation of a long sequence of $\varphi_{32}$ values, for $2 \le b \le 40$, obtained by the Monte Carlo renormalization group (MCRG) method. Our results demonstrate that $\varphi_{32}$, for the studied values of b, monotonically decreases with b, and it seems that for b > 40 the critical exponent $\varphi_{32}$ continues decreasing, and in the limit $b \to \infty$ tends to the Euclidean value $\varphi_{32}^{E} \approx 0$. In addition, using codimension additivity (CA) arguments we have proposed phenomenological formulae for the considered contact critical exponents, and we have tested their predictions on the obtained sets of data. We find that, for fractals labelled with smaller values of b, the CA proposals give satisfactory agreement with existing convincing results.

Based on the findings of the performed investigation we may conclude that the set of obtained results of the studied problem has been significantly extended. We have demonstrated that the statistics of two cross-linked polymer chains on the family of 3D SG fractals can be rewardingly studied by the MCRG method. In particular, the MCRG study of the contact critical exponents revealed their interesting behaviour as functions of the fractal scaling parameter b, making a step forward to prescribing the behaviour of SAW critical exponents in the fractal-to-Euclidean crossover region. As a further investigation one may attempt to extend our study for calculating the contact critical exponent $\varphi_{33}$, when both polymers are floating chains in the bulk of a 3D SG fractal. In addition, to make the studied model more realistic (but more difficult to study), it can be supplemented with additional interactions. For instance, one can introduce the interactions between the bulk floating chain and the sites of the adsorbing surface (to promote the adsorbed phase of the floating chain), as well as the intra-chain interactions (to promote a collapsing phase of the bulk floating chain), and then, in the space of interaction parameters, the phase diagram can be investigated, together with new contact critical exponents at appropriate phase transition fixed points.

## Reference

Zivic, (2007) On the number of contacts of a floating polymer chain cross-linked with a surface adsorbed chain on fractal structures, Journal of Statistical Mechanics: Theory and Experiment, P02005.

## Contact

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