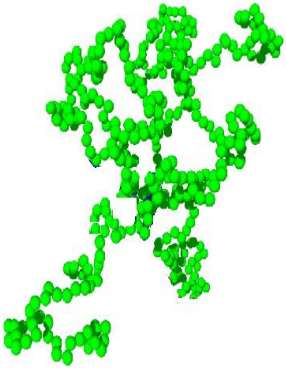
Self-avoiding random walks on percolation clusters: multifractal effects

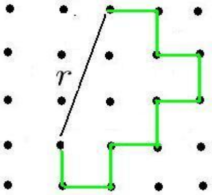
Viktoria Blavatska[1,2], Wolfhard Janke[1]

[1] Institut für Theoretische Physik, Leipzig Universität, Leipzig, Germany
[2] Institute for Condensed Matter Physics, Lviv, Ukraine

Leipzig, 28th November 2008

SAW as a model of polymer chain





- Averaged end-to-end distance: $\langle r \rangle \sim N^{\nu_{\mathrm{SAW}}}$
- ν_{SAW} – universal exponent
- Fractal dimension of SAW: $d_{\mathrm{SAW}} = 1/\nu_{\mathrm{SAW}}$

Methods of study

Numerical simulations: ($N \sim 10^6$)

$\nu_{\rm SAW}(d{=}2){=}0.7496 \pm 0.0001$, $\nu_{\rm SAW}(d{=}3){=}0.5877 \pm 0.0006$ (Li et al., 1995).

Field theory:

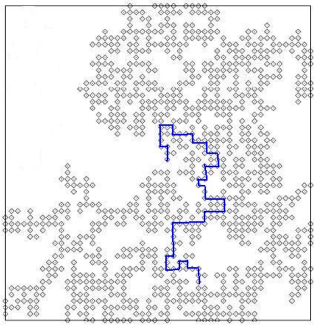
$$\mathcal{H}_{eff} = \int \mathrm{d}^d x \left[\frac{1}{2} \left(\mu^2 |\vec{\varphi}(x)|^2 + |\nabla \vec{\varphi}(x)|^2 \right) + \frac{u_0}{4!} (\vec{\varphi}^2(x))^2 \right],$$

$\vec{\varphi} = \{\varphi^1, \ldots, \varphi^m\}$, polymer limit: $m \to 0$ (P. de Gennes, 1979)

$$\begin{aligned} \nu_{\rm SAW} &= \frac{1}{2} + \frac{\varepsilon}{16} + \frac{15\varepsilon^2}{64} + \ldots, \quad \varepsilon = 4 - d; \\ \nu_{\rm SAW}(d{=}3) &= 0.5882 \pm 0.0011 \end{aligned}$$

(Guida and Zinn Justin, 1998).

SAWs on disordered lattices: Percolation threshold



Critical site concentration: $p = p_c$.

d	2	3	4	5	6
p_c	0.592	0.311	0.196	0.146	0.108

Fractal dimension of percolation cluster:
$\langle \mathcal{N} \rangle \sim L^{d^F_{p_c}}$

d	2	3	4	5	6
$d^F_{p_c}$	$91/49$	2.51	3.05	3.49	4

Upper critical dimension: $d_c = 6$
(Stauffer, Phys. Reports, 1979)

What happens with SAWs' exponents?
$\nu_{p_c}, \gamma_{p_c} = ?$

Methods of study

Field theory (Meir and Harris, 1989):

$$\mathcal{H}_{eff} = \int d^d x \frac{1}{2} \sum_k \left(\mu_k^2 |\varphi_k(x)|^2 + |\nabla \varphi_k(x)|^2\right) + \frac{w}{6} \int d^d x \varphi_{k_1}(x)\varphi_{k_2}(x)\varphi_{k_3}(x)$$

$$\nu_{p_c} = \frac{1}{2} + \frac{\epsilon}{42} + \frac{110\epsilon^2}{21^3} + \ldots, \quad \epsilon = 6 - d$$

$\nu_{p_c}(d{=}2){=}0.785$, $\nu_{p_c}(d{=}3){=}0.671$, $\nu_{p_c}(d{=}4){=}0.595$

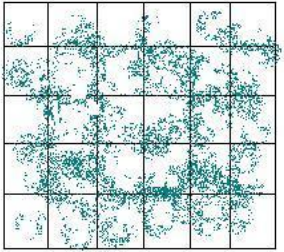
$$\nu^{(q)} = \frac{1}{2} + \left(\frac{5}{2} - \frac{3}{2^q}\right)\frac{\varepsilon}{42} + \left(\frac{589}{21} - \frac{397}{14 \cdot 2^q} + \frac{9}{4^q}\right)\left(\frac{\varepsilon}{42}\right)^2, \quad \varepsilon = 6 - d$$

(Janssen, 2007)

Numerical simulations:

$\nu_{p_c}(d{=}2){=}0.783 \pm 0.003$ (Grassberger, 1993)
$\nu_{p_c}(d{=}3){=}0.667 \pm 0.003$, $\nu_{p_c}(d{=}4){=}0.586 \pm 0.003$ (Blavatska and Janke, 2008)

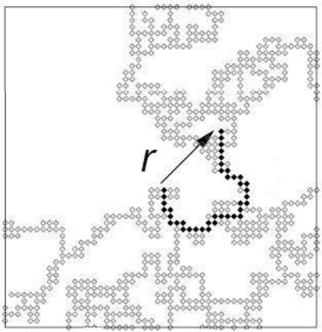
Multifractality



- "Population" of N members is distributed on the surface
- "Measure" of ith cell: $p_i = N_i/N$
- Multifractal moments: $M^{(q)} = \sum_i p_i^q \sim L^{\tau(q)}, \quad \tau(q) \neq q \cdot \tau(1)$
- Singularities with Hölder exponents α: $p_j \sim L^{-\alpha}$
- Number of cells with singularity α: $\mathcal{N}(\alpha) \sim L^{f(\alpha)}$
- $f(\alpha)$ – spectral function, set of fractal dimensions
- $\alpha(q) = \frac{\mathrm{d}\tau(q)}{\mathrm{d}q}, \quad f(\alpha) = q\alpha - \tau(q)$

(Hentschel and Procaccia, Physica D 1983)

Backbone of the percolation cluster

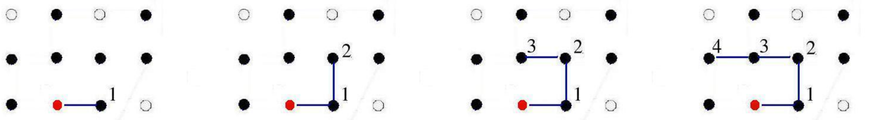


- Cutting off “dead ends”
- Geometrical backbone - fractal object:

$$\langle \mathcal{N} \rangle \sim L^{d^B_{p_c}}$$

d	2	3	4
ν_{min}	0.884	0.727	0.638
$d^B_{p_c}$	1.650	1.86	1.95

Pruned-enriched Rosenbluth method (PERM)



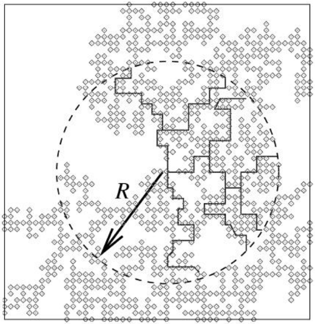
Weight of Nth step: $W_N = \prod_{l=1}^{N} w_l$ (algorithm of Rosenbluth)

Configurational averaging: $\langle(\cdots)\rangle = \frac{\sum_{conf} W_N(\cdots)}{Z}, \; Z = \sum_{conf} W_N$

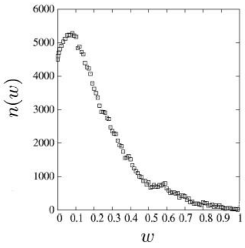
Control parameters: $W_n^{max} = c_1 Z_n/Z_1, \quad W_n^{min} = c_2 Z_n/Z_1$ (Grassberger, 1997)

- $W_n < W_n^{min}$ – pruning with probability $1/2$, $W_n = 2W_n$
- $W_n > W_n^{max}$ – enrichment, $W_n = W_n/2$

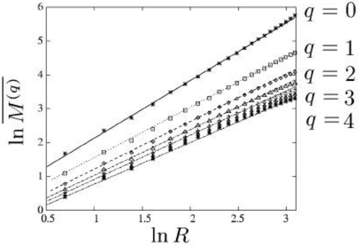
SAW on percolation clusters: Multifractality



- $L(R)$ - number of SAW trajectories with fixed distance R between end points
- $L(x)$ - number of trajectories, passing through a site x
- $w(x) = L(x)/L(R)$ - “weight” of the site x
- Weight distribution:



Multifractal moments



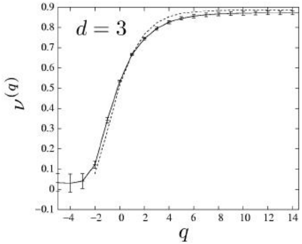
- $d = 2, 3, 4$ - dimensional lattices
- $L = 500, 200, 50$ – maximum lattice size
- $R \leq L/3$ – to avoid finite-size effects
- Multifractal moments:

$$M^{(q)}(R) = \sum_x w^q(x)$$

- Averaging over disorder:

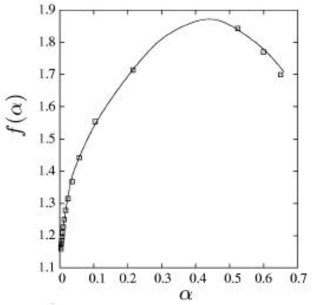
$$\overline{M^{(q)}(R)} \sim R^{1/\nu^{(q)}}$$

Spectrum of multifractal exponents



- RG result:
  $\nu^{(q)}=\frac{1}{2}+\left(\frac{5}{2}-\frac{3}{2^q}\right)\frac{\varepsilon}{42}+\left(\frac{589}{21}-\frac{397}{14\cdot 2^q}+\frac{9}{4^q}\right)\left(\frac{\varepsilon}{42}\right)^2$
  $\varepsilon = 6 - d$
  (Janssen and Stenull, Phys. Rev. E 2007)
- Our numerical estimates:
- $q = 0: \ \nu^{(0)} = 1/d^B_{p_c} = 0.532 \pm 0.007 (d = 3)$
- $q = 1: \ \nu^{(1)} = \nu_{p_c} = 0.669 \pm 0.007 \ \ (d = 3).$
- $q \to \infty$: “red sites” mainly contribute:
  $N_{\rm red} \sim R^{\nu_p}$
  ν_p – percolation correlation length exponent
  $\nu^{(\infty)} = \nu_p = 0.852 \ (d = 3)$

Spectral function

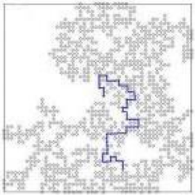


- Set of sites x_i with $w(x_i) \sim R^{-\alpha}$, $\alpha_{\min} < \alpha < \alpha_{\max}$
- Number of sites $N_R(\alpha) \sim R^{f(\alpha)}$
- $f(\alpha)$ – frequency of observation of a particular value of α
- $f(\alpha) = q\alpha - \tau(q)$, $\alpha(q) = \frac{\partial \tau(q)}{\partial q}$ with $\tau(q) = 1/\nu^{(q)}$.
- $\alpha_{\min} = \lim_{q \to +\infty} \tau(q)/(q-1)$, $\alpha_{\max} = \lim_{q \to -\infty} \tau(q)/(q-1)$
- The maximum value of $f(\alpha)$ gives the fractal dimension of the underlying structure $d^B_{p_c}$

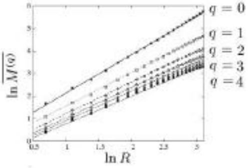
(V. Blavatska, W. Janke, Phys. Rev. Lett. 2008)

Conclusions

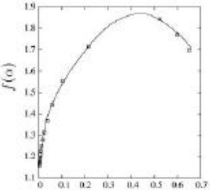
- SAW reflects universal properties of polymer chain



- Percolation threshold: new universality class



- Multifractal exponents



- Spectrum of singularities