

Random walks in power-law correlated disordered environments

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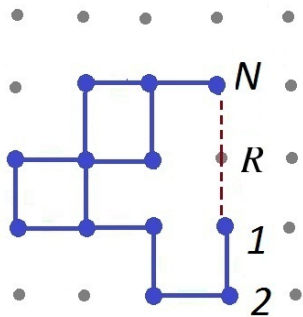
in cooperation with

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and Wolfhard Janke²

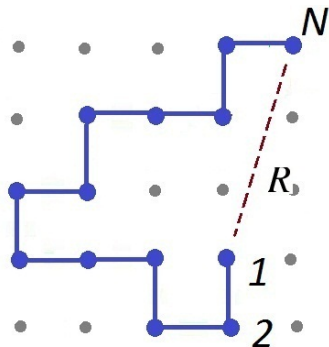
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Random Walks (RWs)



Self-Avoiding Walks (SAWs)

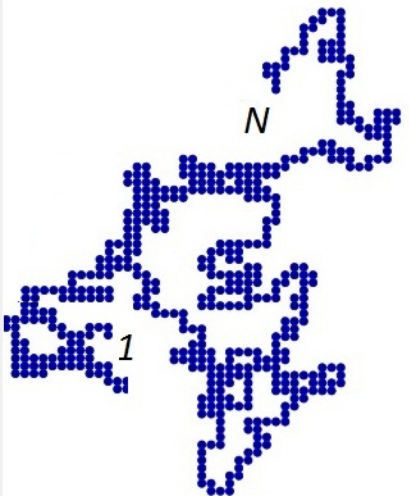
End-to-end distance: $\langle R^2 \rangle \sim N^{2\nu}$

Universal size exponent ν :

$$\nu_{\text{RW}} = \frac{1}{2}$$

$$\nu_{\text{SAW}} = \frac{3}{d+2}$$

Definitions: Gyration tensor

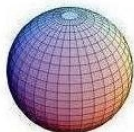


- Position vectors $\vec{R}_n = \{x_n, y_n\}$, $(n = 1, \dots, N)$.
- Center of mass \vec{R}_{CM} with $x_{CM} = \frac{\sum_{n=1}^N x_n}{N}$, $y_{CM} = \frac{\sum_{n=1}^N y_n}{N}$.
- Gyration tensor

$$Q_{xy} = \frac{1}{N} \sum_{n=1}^N (x_n - x_{CM})(y_n - y_{CM})$$

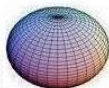
- Eigenvalues λ_i measures the **shape**

Definitions: Gyration tensor



$$\lambda_1 = \lambda_2$$

$$A = 0$$



$$0 < A < 1$$



$$\lambda_1 \neq 0, \lambda_2 = 0$$

$$A = 1$$



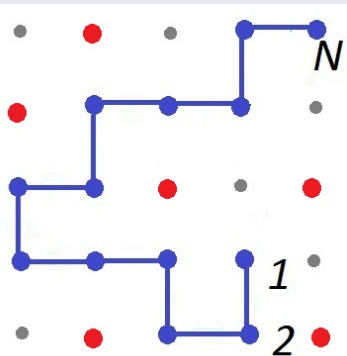
Random walk trajectories are **asymmetrical** (W. Kuhn (1934); K. Solc and W.H. Stockmayer (1971))

Rotational invariant: **Asphericity** $A = \frac{1}{d(d-1)} \sum_{i=1}^d \frac{(\lambda_i - \bar{\lambda})^2}{\bar{\lambda}^2} = \frac{d}{d-1} \frac{\text{Tr} \hat{\mathbf{Q}}^2}{(\text{Tr} \mathbf{Q})^2}$

with $\bar{\lambda} \equiv \frac{1}{N} \sum_{i=1}^d \lambda_i = \frac{1}{N} \text{Tr} \mathbf{Q}$, $\hat{\mathbf{Q}} \equiv \mathbf{Q} - \text{Tr} \mathbf{Q} \mathbf{I}$ (J.A. Aronovitz and D.R. Nelson, *J. Physique* **47** 1445 (1986).)

- **Random walk:** $A_{RW}(d=2) = 0.392 \pm 0.005$ (J. Rudnick and G. Gaspari, *J. Phys. A* **19**, L191 (1986))
- **Self-avoiding walk:** $A_{SAW}(d=2) = 0.501 \pm 0.003$ (M. Bishop and C.J. Saltiel, *J. Chem. Phys.* **88** (1988))

Random-walks in disordered environment



- ● - site with defect
- p – concentration of disorder
- uncorrelated point-like defects: universal size and shape characteristics are not altered unless $p > p_c$
(Y. Kim, J. Phys. C 16, 1345 (1983);
S. B. Lee and H. Nakanishi, Phys. Rev. Lett. 61, 2022 (1988).)
- p_c - percolation threshold
- $p_c(d = 2) = 0.407$
(R.M. Ziff, Phys. Rev. Lett. 72, 1942 (1942).)

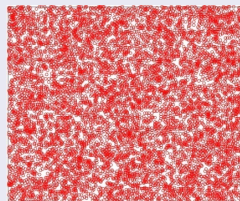
Long-range correlated disorder

- Defects are correlated on large distances r according to a power law with a pair correlation function

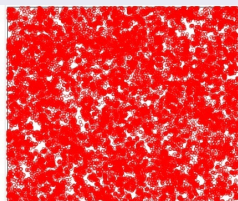
$$C(r) \sim r^{-a}$$

(A. Weinrib and B.I. Halperin, *Phys. Rev. B* **27**, 413 (1983))

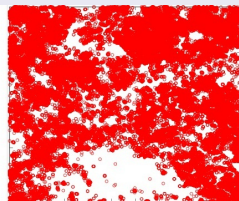
- $a = d$ – uncorrelated point-like defects
- $a < d$ – defects in the form of extended fractal clusters
- Fourier filtering method (FFM) (S. Prakash et al., *Phys. Rev. A* **46** (1992); H.A. Makse et al., *Phys. Rev. E* **53** (1996))



$a=2.0$

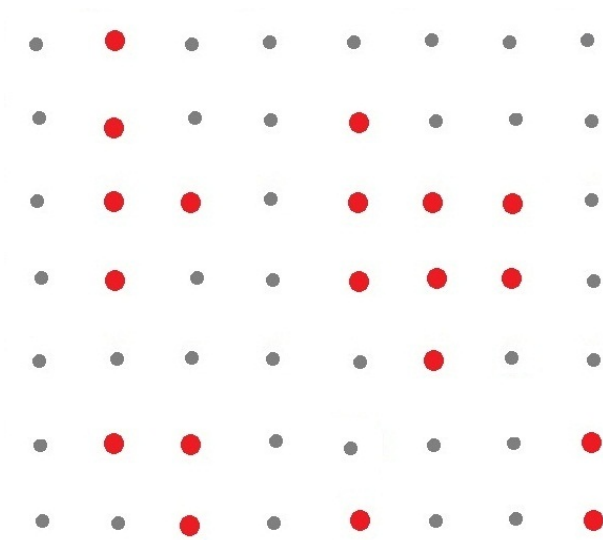


$a=1.8$

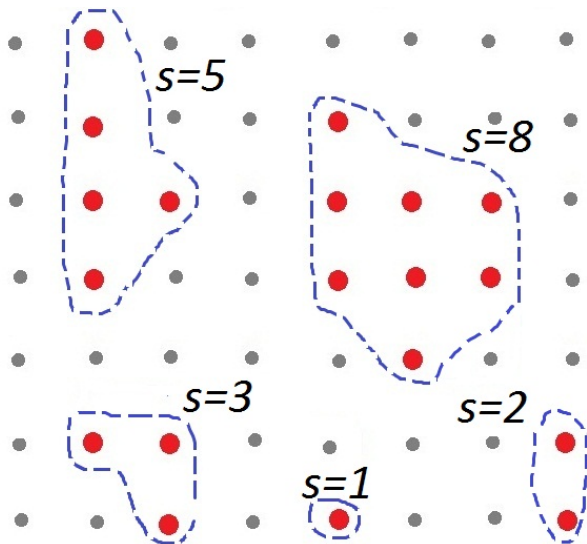


$a=0.25$

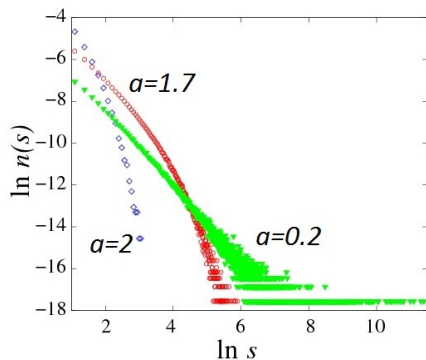
Cluster size distribution



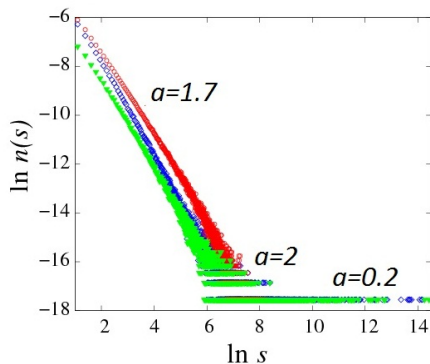
Cluster size distribution



Cluster size distribution

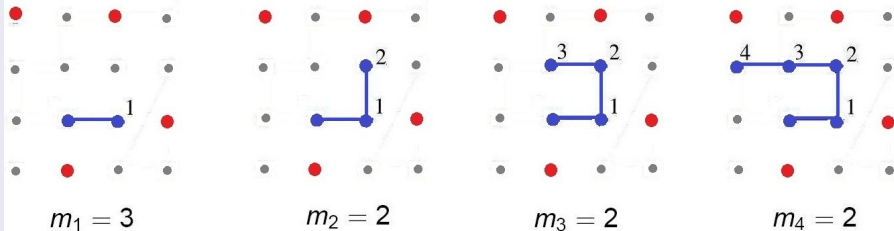


20 % of disorder



50 % of disorder

Pruned-enriched Rosenbluth method (PERM)



Weight of N th step: $W_N = \prod_{l=1}^N m_l$ (M.N. Rosenbluth, *J. Chem. Phys.* **23**, 356 (1955))

Control parameters: W_n^{max} W_n^{min} (P. Grassberger, *Phys. Rev. E* **56**, 3682 (1997))

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

Observables averaging

The **configurational averaging** for any observable O :

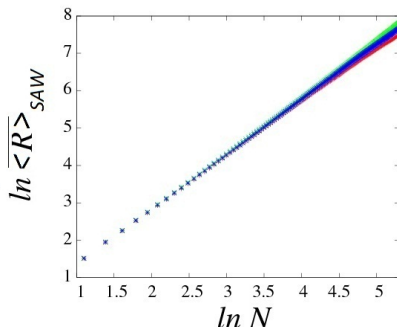
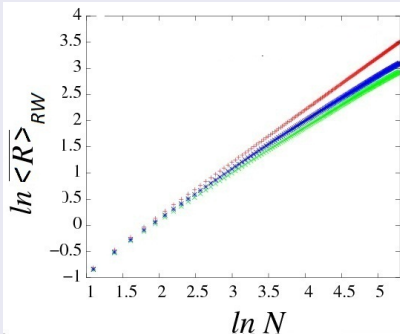
$$\langle O \rangle = \frac{\sum_{\text{conf}} W_N^{\text{conf}} O}{\sum_{\text{conf}} W_N^{\text{conf}}}, \quad (1)$$

The **averaging over different realizations of disorder**, i.e., over different constructed disordered lattices

$$\overline{\langle O \rangle} = \frac{1}{M} \sum_{i=1}^M \langle O \rangle_i. \quad (2)$$

We consider $M = 1000$ configurations of disorder in $d = 2$ -dimensional lattices of linear size 2048×2048 at various values of correlation parameter a .

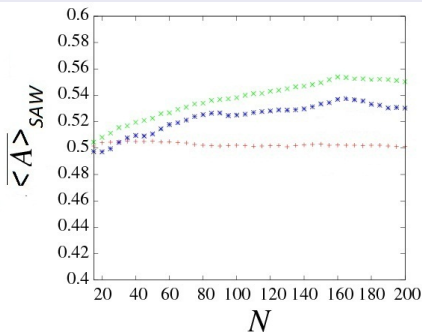
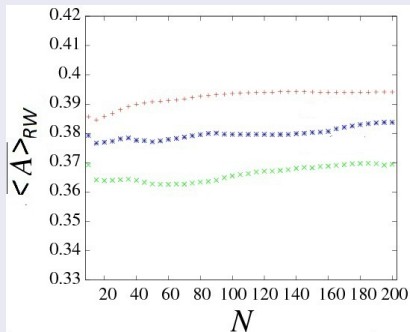
Size exponent



Averaged end-to-end distance of RW and SAW on a lattice with 20% of disorder at $a = 2.0$, $a = 1.75$, $a = 0.25$

a	ν_{RW}	ν_{SAW}
2.0	0.5 ± 0.001	0.750 ± 0.001
1.75	0.482 ± 0.001	0.757 ± 0.001
0.25	0.470 ± 0.001	0.764 ± 0.001

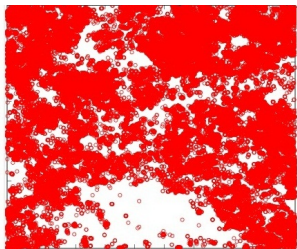
Asphericity



Averaged asphericity of RW and SAW on a lattice with 20% of disorder at
 $a = 2.0$, $a = 1.75$, $a = 0.25$

a	$\langle A \rangle_{RW}$	$\langle A \rangle_{SAW}$
2.0	0.393 ± 0.002	0.501 ± 0.003
1.75	0.380 ± 0.002	0.538 ± 0.003
0.25	0.370 ± 0.002	0.546 ± 0.003

Conclusions



- Defects are correlated on large distances r according to a power law with a pair correlation function

$$C(r) \sim r^{-a}$$

- The RWs are more compact and symmetric in correlated environments
- The SAWs are more extended and asymmetric in correlated environments

