Polymers in crowded environment under stretching force: globule-coil transitions

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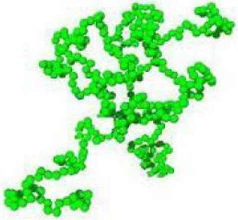
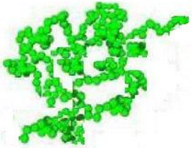
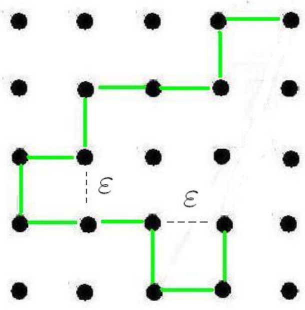
Configurations of polymer macromolecule





$T > \color{red}{T_\Theta}$	$T = \color{red}{T_\Theta}$	$T < \color{red}{T_\Theta}$
polymer coil	*tricritical point*	*globule*
$\langle R^2 \rangle \sim N^{2\nu_{\rm SAW}}$,	$\langle R^2 \rangle \sim N^{2\nu_\Theta}$,	$\langle R^2 \rangle \sim N^{2/d}$
$\nu_{\rm SAW}(d=2) = 3/4$,	$\nu_\Theta(d=2) = 4/7$,	
$\nu_{\rm SAW}(d=3) = 0.588$	$\nu_\Theta(d \geq 3) = 1/2$	

Self-attracting self-avoiding walks (SASAW)



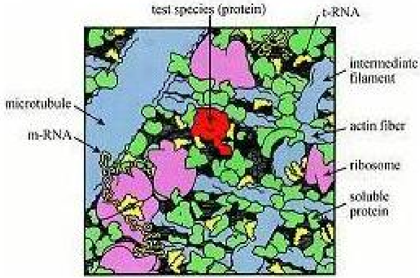
- Statistical weight: $W_N \sim \mathrm{e}^{\frac{-E_N}{k_B T}}$
- $E_N = n \cdot \varepsilon$ – energy of a chain
- n – number of nearest neighbour contacts
- let us take: $k_B = 1$, $\varepsilon = -1$

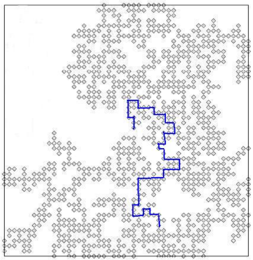
d	μ	T_Θ
2	2.6385(1)[a]	1.499(2)[c]
3	4.68404(9)[b]	3.717(3)[d]

- μ – connectivity constant

[a]: A.J. Guttmann, J. Phys. A **24** (1991)
[b]: D. MacDonald, J. Phys. A **33** (2000)
[c]: G.T. Barkema, J. Stat. Phys. **90** (1998)
[d]: P. Grassberger, Phys. Rev. E **56** (1997)

SASAW in crowded environment



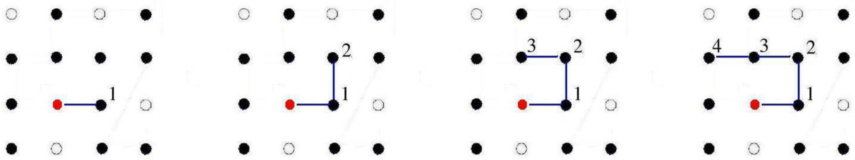


$p \simeq 40\%$ (A. Minton, J. Biol. Chem. **276**, 2001)

- p – concentration of lattice sites, allowed for SAW
- percolation cluster at critical concentration p_c

d	2	3	4
p_c	0.592	0.311	0.196

Pruned-enriched Rosenbluth method (PERM)



$m_1 = 3$ $m_2 = 2$ $m_3 = 2$ $m_4 = 2$

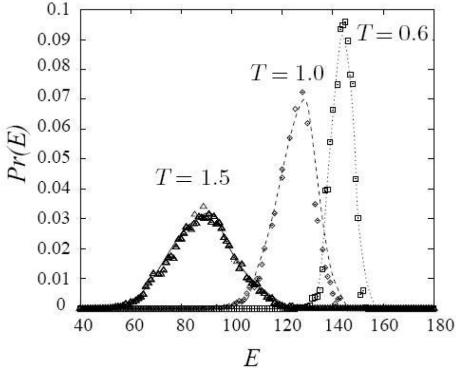
Weight of Nth step: $W_N = \prod_{l=1}^{N} w_l e^{\frac{-(E_N - E_{N-1})}{k_B T}}$

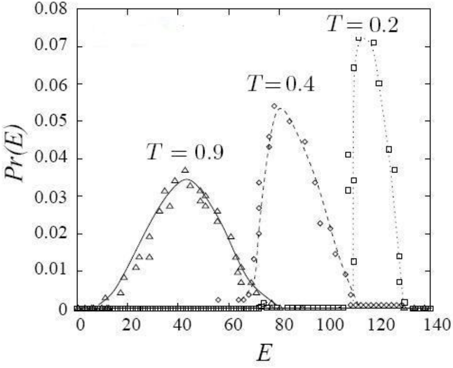
Control parameters: W_n^{max} W_n^{min} (Grassberger'97)

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

Percolative lattice: $L = 400 (d = 2)$, $L = 200 (d = 3)$

Energy distributions



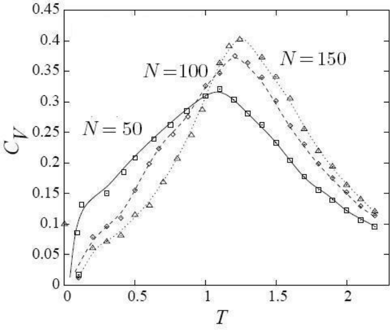


$d = 2$, pure lattice
$T_\Theta \sim 1.5$

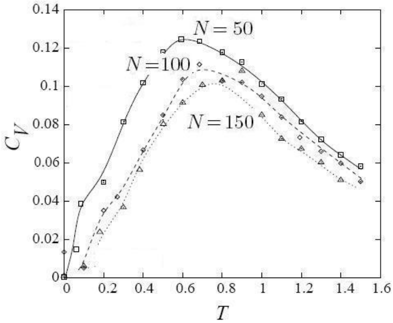
$d = 2$, percolation cluster
$T_\Theta^{p_c} \sim 0.9$

Heat capacity

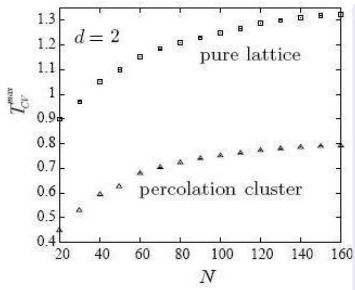
$$C_V(T) = \frac{1}{T^2}\left(\overline{\langle E^2\rangle} - \overline{\langle E\rangle^2}\right).$$

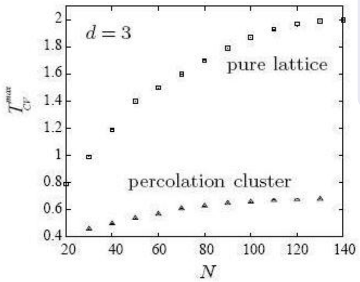


$d = 2$, pure lattice



$d = 2$, percolation cluster





- $T_{C_V}^{\max}(N) < T_\Theta$ at finite N,

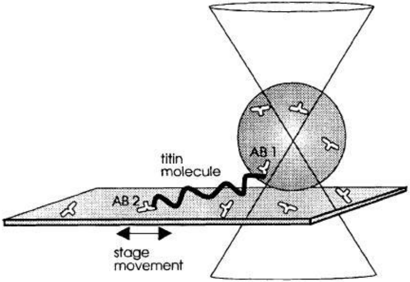
$$T_{C_V}^{max}(N) - T_\Theta \sim N^{-\nu_\Theta}$$

- $d = 2$, pure lattice: $\nu_\Theta = 4/7$[a]
- $d = 2$, pc: $\nu_\Theta^{p_c} = 0.74(2)$[b]
- $d = 3$, pure lattice: $\nu_\Theta = 1/2$
- $d = 3$, pc: $\nu_\Theta^{p_c} = 0.60(2)$[b]

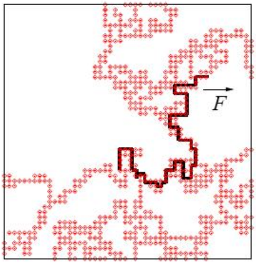
d	μ_{p_c}	$T_\Theta^{p_c}$ (our study)
2	1.565(2)[c]	0.92(2)
3	1.462(2)[c]	0.71(2)

[a]: B. Duplantier, Phys. Rev. Lett. **59** (1982)
[b]: K. Barat, J. Phys. A **25** (1992)
[c]: A. Ordemann, Phys. Rev. E **61** (2000)

Polymers under stretching force

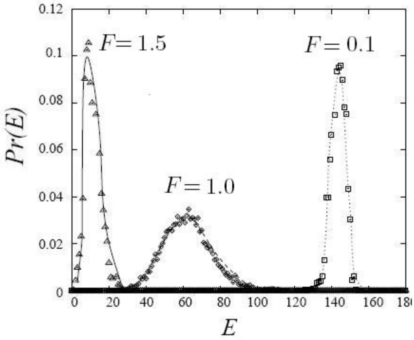


(M. Rief, Science **276** 1997)

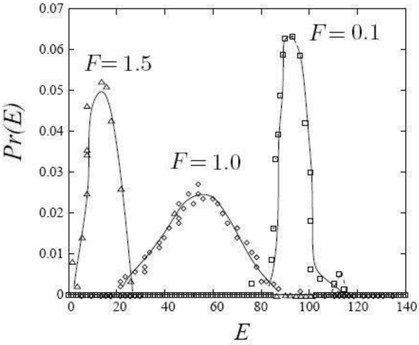


- Statistical weight of SASAW under force F: $W_N \sim \mathrm{e}^{\frac{-E_N - E_s}{k_B T}}$
- $E_N = n \cdot \varepsilon$ – interaction energy of a chain
- $E_s = -Fx$ – stretching energy, $x = |x_N - x_0|$ – extention
- pure: Grassberger'2002, Marenduzzo'2003;
  disorder: Kumar'2009 ($d = 2$)

Energy distributions



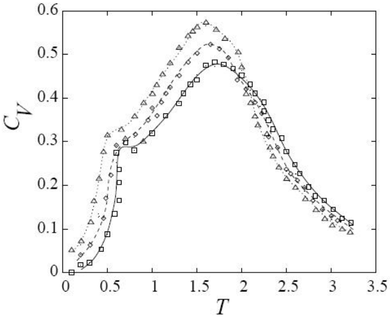
$d = 2$, pure lattice
$T = 0.4 < T_\Theta$



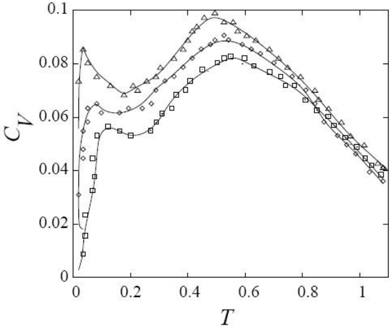
$d = 2$, percolation cluster
$T = 0.1 < T_\Theta$

Heat capacity

$$C_V(T) = \frac{1}{T^2}\left(\overline{\langle E^2\rangle} - \overline{\langle E\rangle^2}\right).$$



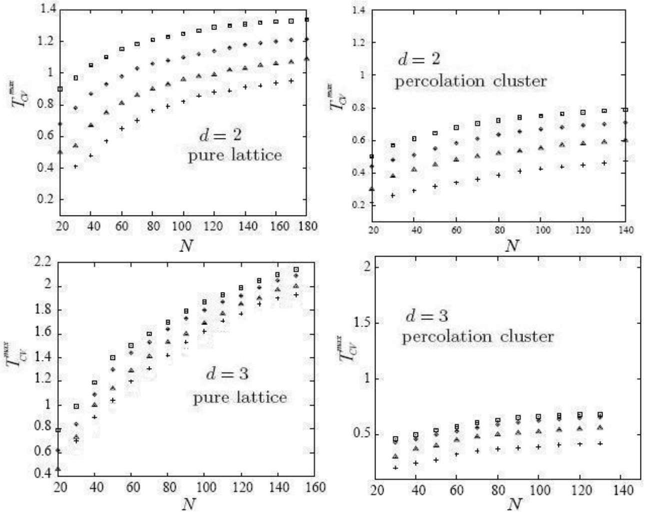
$d = 3$, pure lattice



$d = 3$, percolation cluster

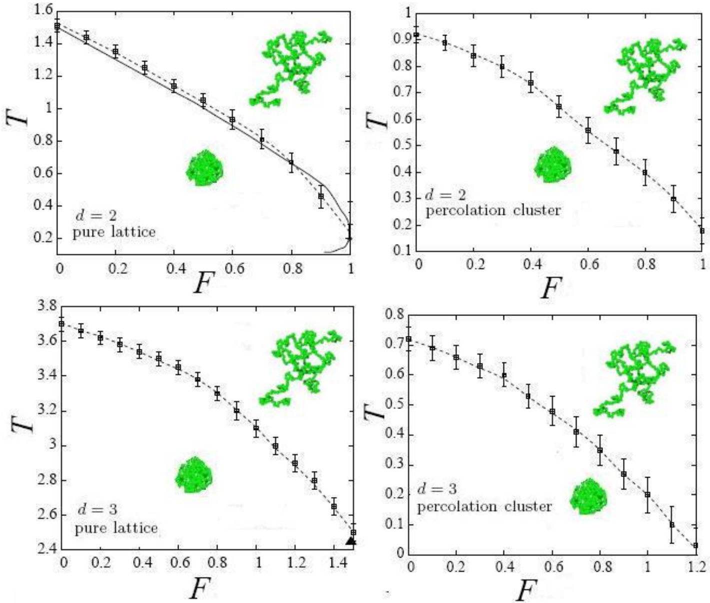
Squares: $F = 0.2$, diamonds: $F = 0.4$, triangles: $F = 0.6$.

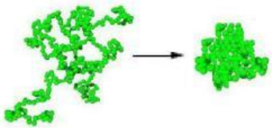
Analysis of specific-heat peaks

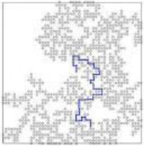


Squares: $F=0$, diamonds: $F=0.2$, triangles: $F=0.4$, pluses: $F=0.6$.

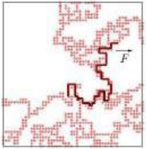
Globule-coil transitions under stretching force







Estimations of globule-coil transition temperature $T_{\Theta}^{p_c}$ of SASAW on percolative lattices in $d = 2$, $d = 3$



Analyze of applied stretching force on the globule-coil transition of SASAW

Estimations of transition temperature $T_{\Theta}^{p_c}$ under the acting force in environment in $d = 2$, $d = 3$