Knots in Polymers

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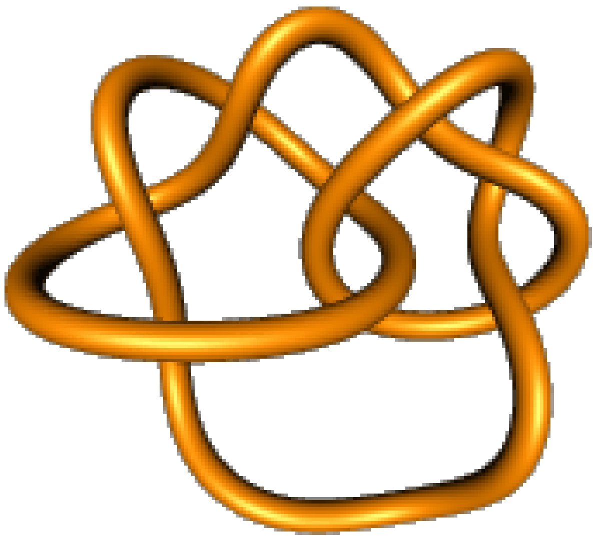
Tel Aviv University



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Oded Farago, UCSB

Roya Zandi, UCLA

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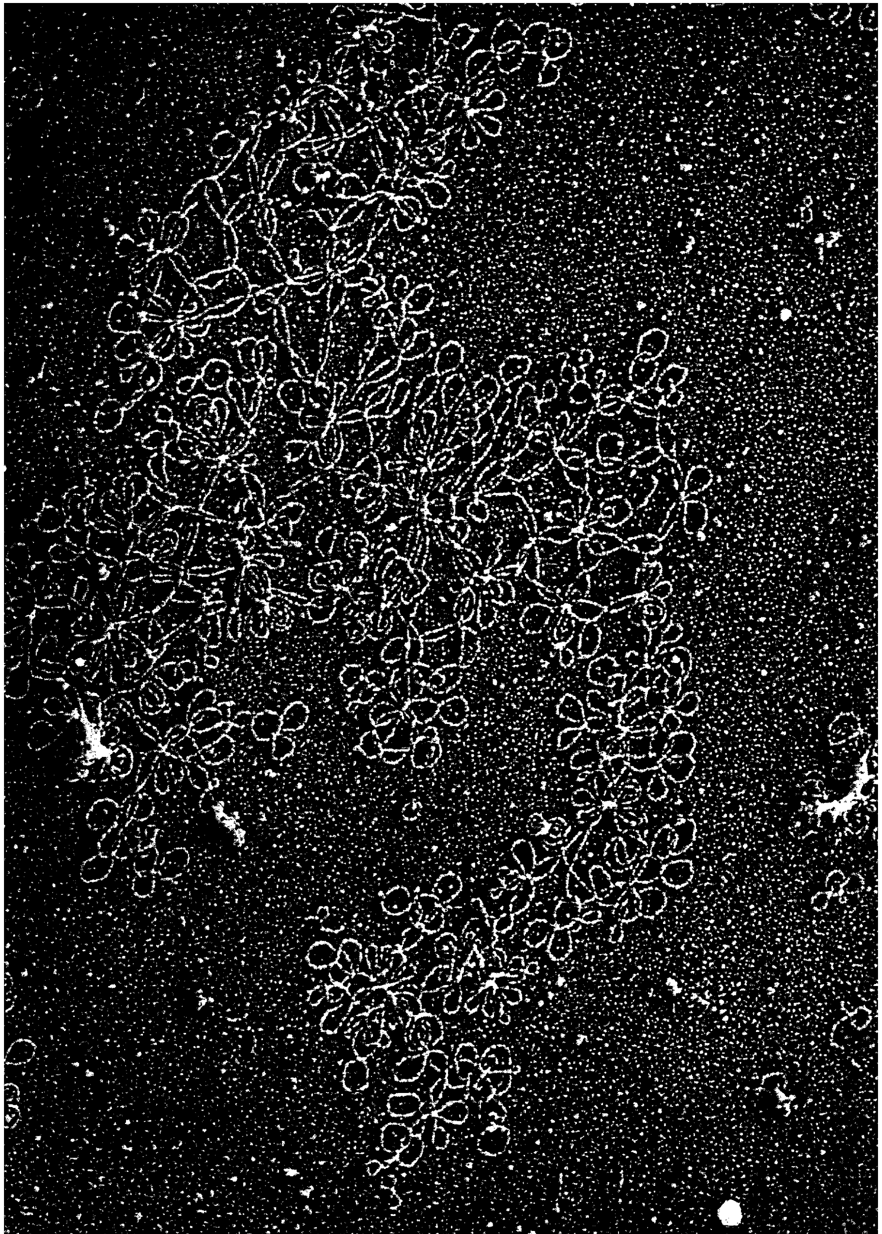
OUTLINE

- *Why knots? Entanglements in macromolecules*
- *Size of a knot – definition of the problem*
- *Knots in charged polymers*
- *Simplified topologies*
- *Force-extension relations and knot sizes*
- *Conclusions*

Entanglements in DNA



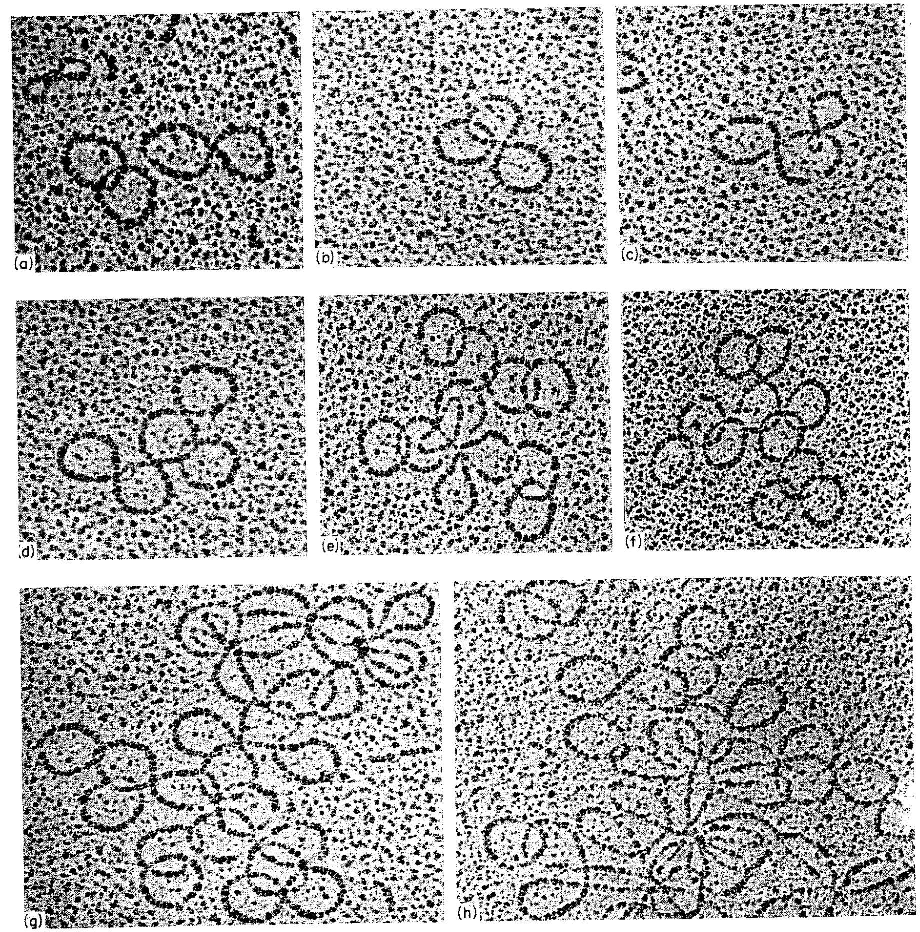
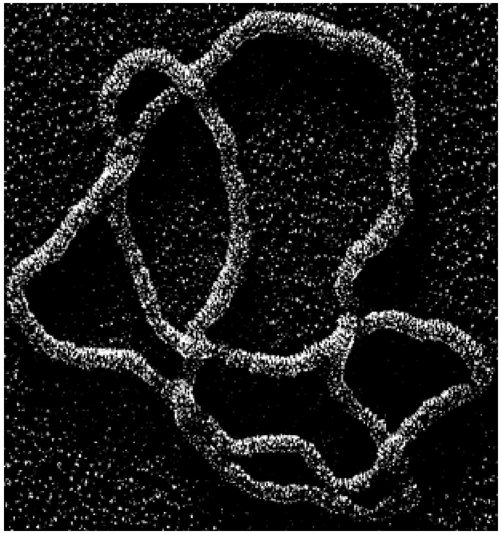


PLATE II. Electron micrographs of different molecular configurations seen in K-DNA. The contour length of a minicircle or one loop of a figure 8 is equal to 0·29 μ.

L.Simpson, A. da Silva
J.Mol.Biol. **56**, 443 (1971)

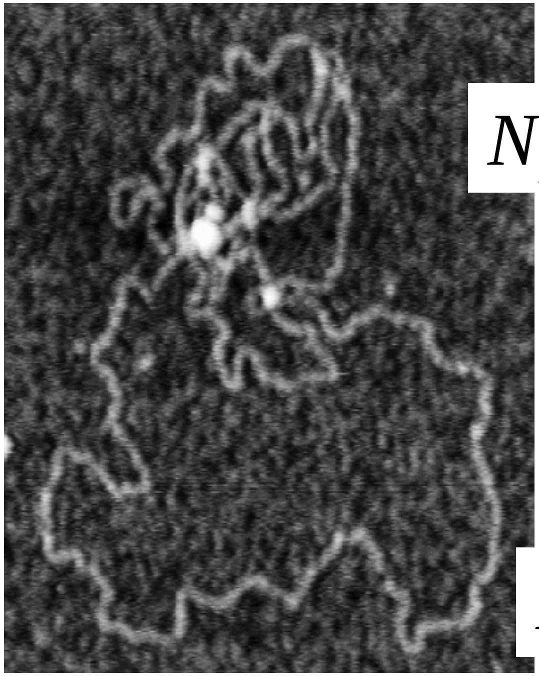
Knots in polymers – reality and statistical mechanics



DNA knot 6_2

Wasserman, Dungan, Cozarelli, Science 229 (85)

How big are the knots?



G. Dietler's group at EPFL

N_k monomers in the knotted region

N total number of monomers

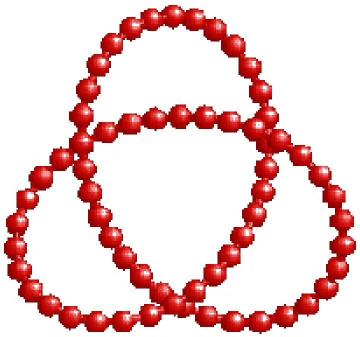
N_k = const   localized

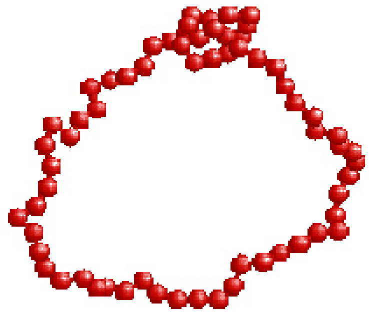
$N_k \sim N^t$, $0<t<1$

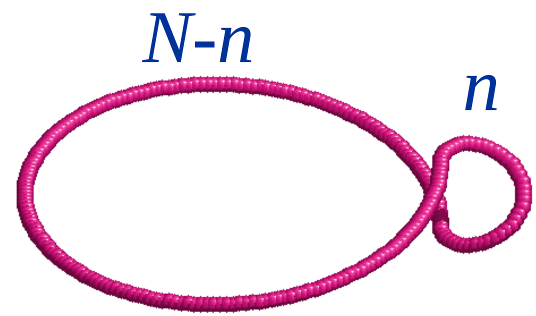
weakly localized

$N_k \sim N$ delocalized

Charged knots







$$E_c(N) = \varepsilon_o \left[N \ln\left(\frac{R}{a}\right) + c\,\frac{aN^2}{R} \right]$$

$$\varepsilon_o \equiv e^2 / \varepsilon a$$

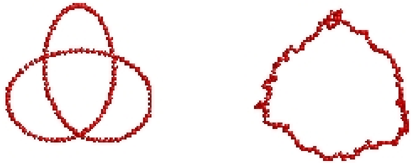
$$E_{\text{TOT}} = E_c(N-n) + E_c(n) + E_{\text{int}}$$

$$E_{\text{int}} = 2\varepsilon_o \left[\ln(N/n) + c' \right]$$

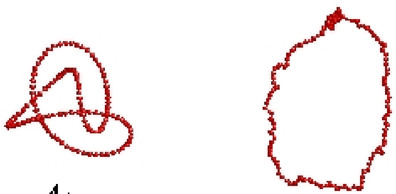
$$E_{\text{TOT}} = const. + \varepsilon_o n \ln(N/n)$$

Dommersnes, Kantor, Kardar, PRE 66 (02)

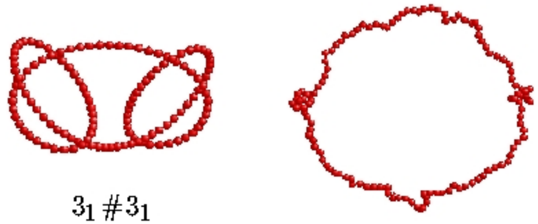
Charged knots (cont'd)



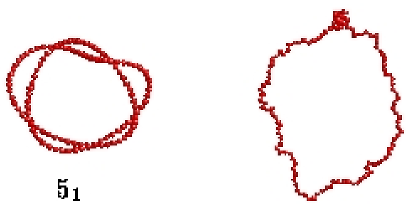
3_1



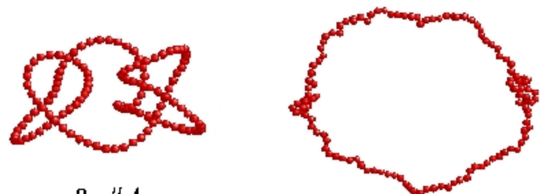
4_1



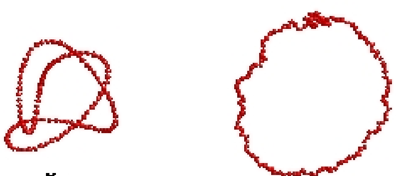
$3_1 \# 3_1$



5_1

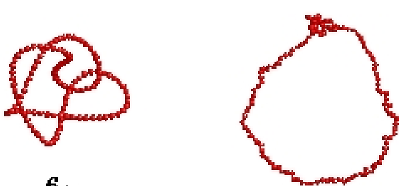


$3_1 \# 4_1$

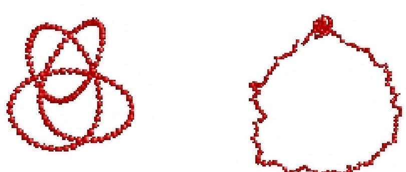


5_2

$3_1 \# 3_1 \# 3_1$

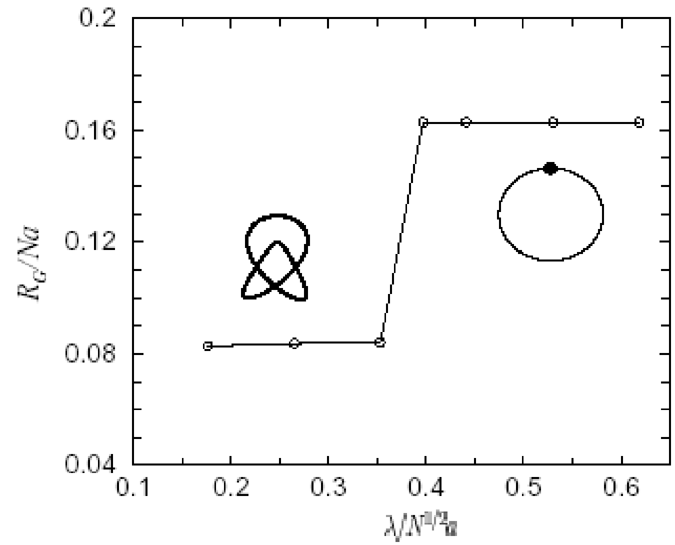


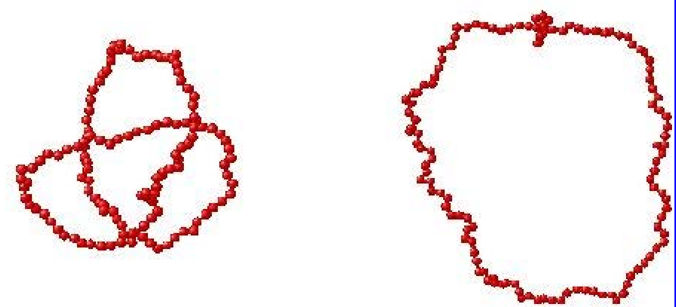
6_1



8_{19}

Screened potential
screening length λ

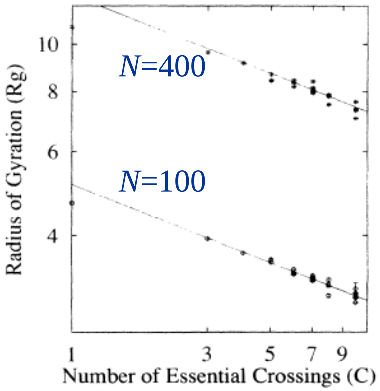




Dommersnes, Kantor, Kardar, PRE 66 (02)

Are knots important? How big are they? (cont'd)

Complexity of a knot influences its radius of gyration.



$C = \#$ of essential crossings

$$R_g \approx a N^{3/5} c^{-4/15}$$

Quake, PRL73 (94)

Grosberg, Feigel, Rabin PRE54 (96)

The radius of gyration of very long polymers is independent of topology.

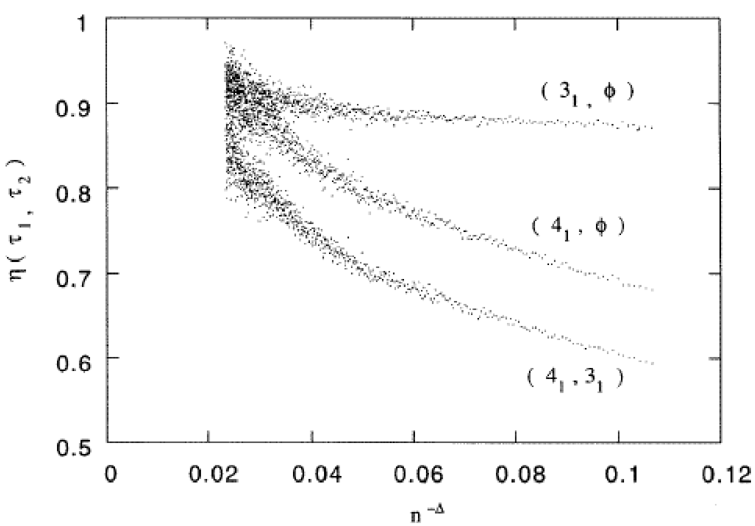
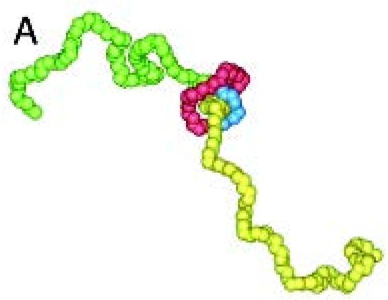
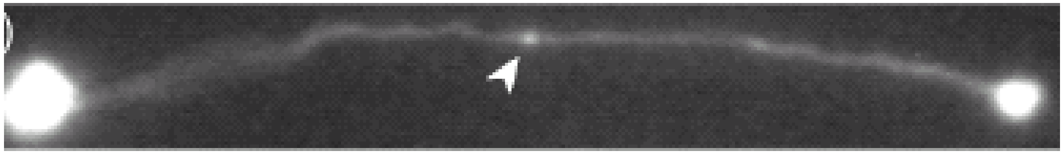


Figure 8. The ratio $\eta(\tau_1, \tau_2) = \langle R_n^2(\tau_1)\rangle / \langle R_n^2(\tau_2)\rangle$ versus $n^{-\Delta}$ for the following pairs of knots: $\tau_1 = 3_1, \tau_2 = \emptyset$; $\tau_1 = 4_1, \tau_2 = \emptyset$; $\tau_1 = 4_1, \tau_2 = 3_1$. All the data points seem to approach 1 as $n \to \infty$.

Janse van Rensburg, Wittington J.Phys. A24 (91)
Orlandini, Tesi, Janse van Rensburg, Wittington J.Phys. A31 (98)

Can we talk about the "size" of a knot "in general"?



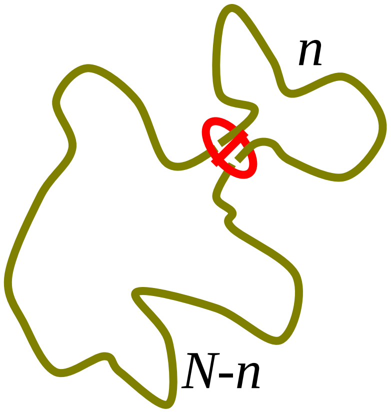


Kim, Klein Macromol. 37 (04)

Bao, Lee, Quake, PRL 91 (03)

Katrich, Olson, Vologodskii, Dubochet, Stasiak PRE61 (00)

Slip link – a substitute for a knot



For Gaussian loops

$$P(N-n)P(n) \sim (N-n)^{-d/2} n^{-d/2}$$

$$\langle n_< \rangle \sim N^{2-d/2} \rightarrow N^{1/2}, \text{ for } d=3$$

Metzler, Hanke, Dommersnes, Kantor, Kardar, PRE 65 (02)

Slip-links in self-avoiding chains

$$P(N,n) \sim (N-n)^{-d\nu} n^{-c}$$

$$d=3 \qquad c=2.23$$

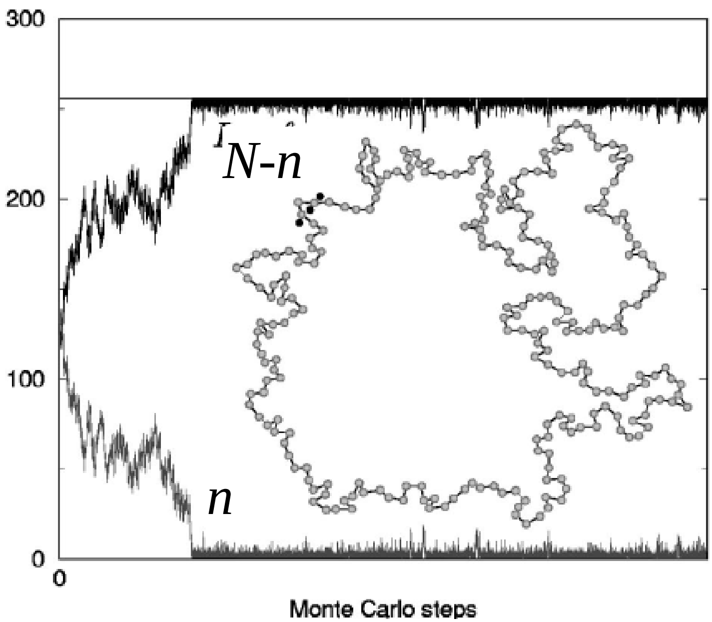
$$d=2 \qquad c=2.6875$$

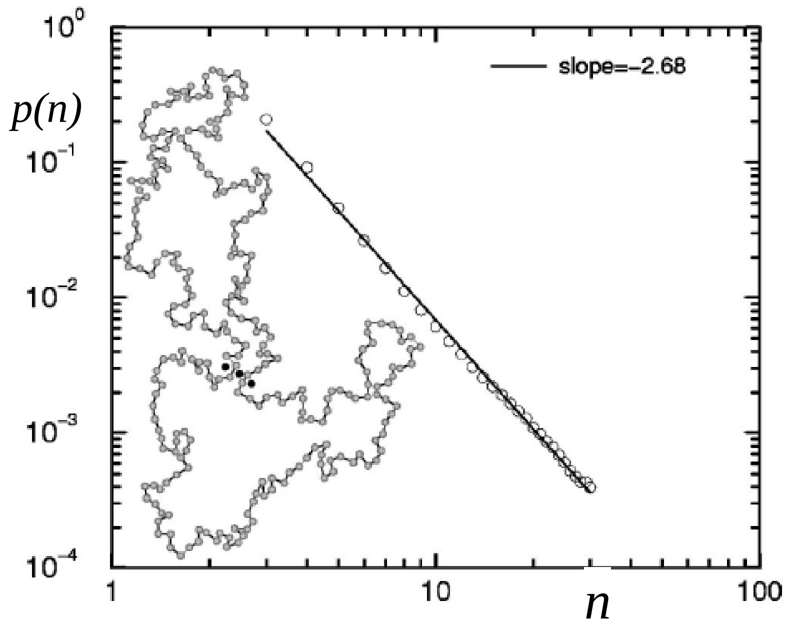
Duplantier PRL 57 (86); J.Stat.Phys.54 (89)
Schafer et al Nucl. Phys. B374 (92)
Ohno, Binder J.Physique 49 (88)

$1<c<2$ weak localization with $t=2-c$ $\qquad (N_k \sim N^{t})$

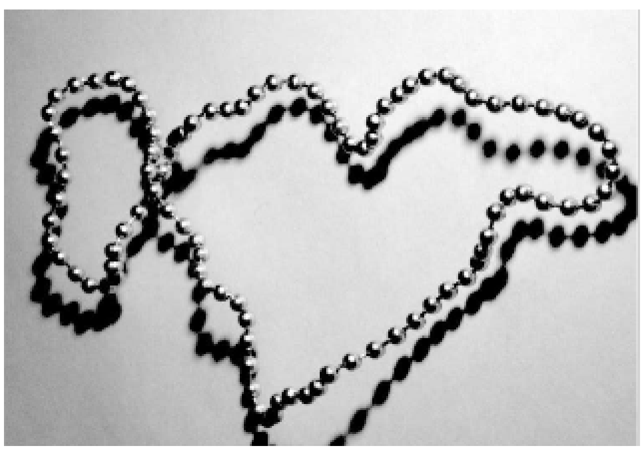
$c>2$ strong localization

Slip-links in self-avoiding chains

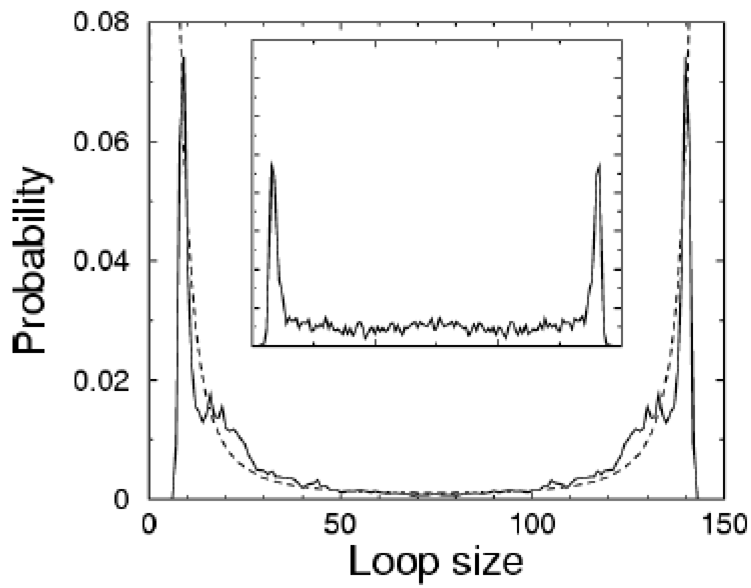




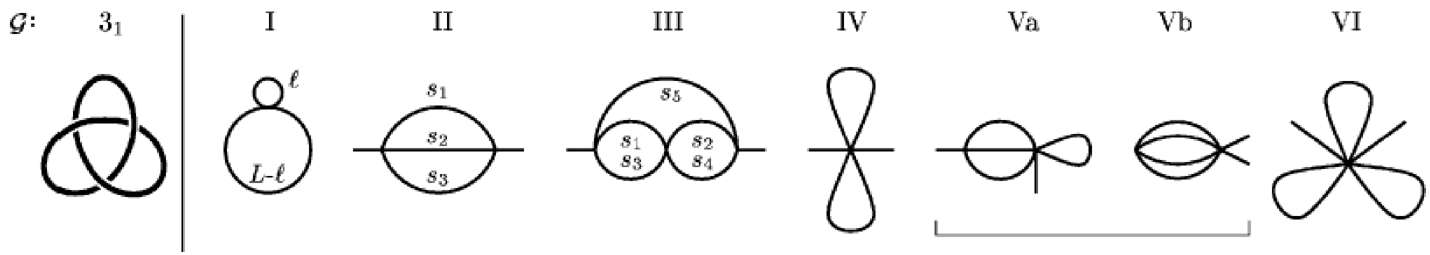
Metzler, Hanke, Dommersnes, Kantor, Kardar, PRE 65 (02)



Hastings, Daya, Ben-Naim, Ecke, PRL (02)



"2D knots"



	I	II	III	IV	Va, Vb	VI
c	$\frac{43}{16}=2.6875$	$\frac{54}{16}=3.375$	$\frac{65}{16}=4.0625$	$\frac{88}{16}=5.5$	$\frac{99}{16}=6.1875$	$\frac{145}{16}=9.0625$

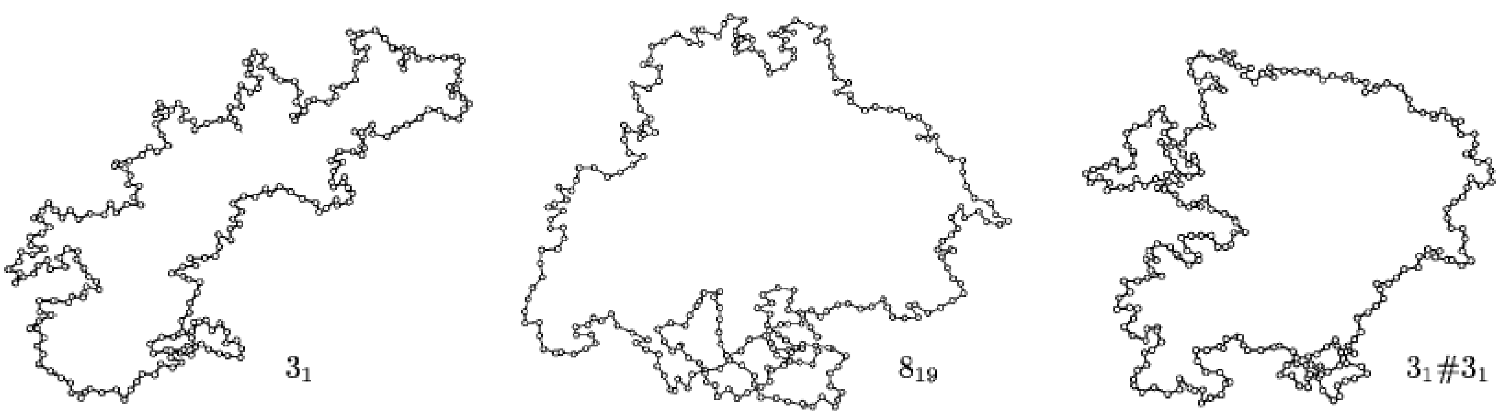
Metzler, Hanke, Dommersnes, Kantor, Kardar, PRL 88 (02)

$$P(N,n)\sim(N-n)^{-d\nu}\,n^{-c}$$

Duplantier PRL 57 (86); J.Stat.Phys.54 (89)
Schafer et al Nucl. Phys. B374 (92)
Ohno, Binder J.Physique 49 (88)

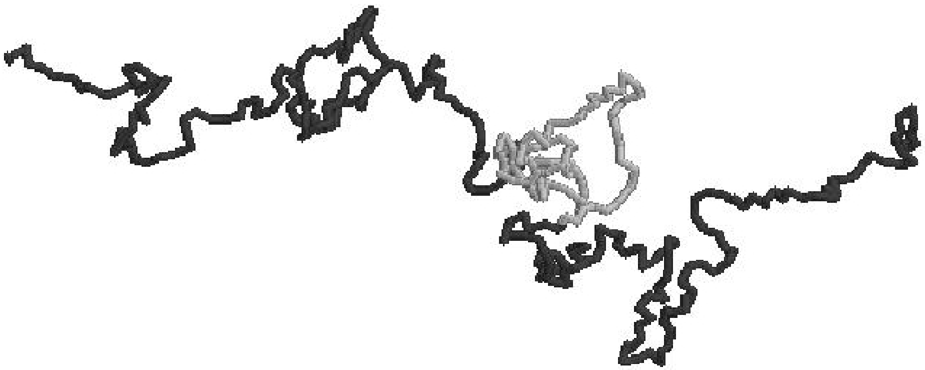
$$(d=2)\qquad c=\sum_{N\geq 4} m_N\left[\frac{N}{2}(d\nu-1)+(|\sigma_N|-d\nu)\right]$$

N – number of "legs" at junction
m – number of such junctions



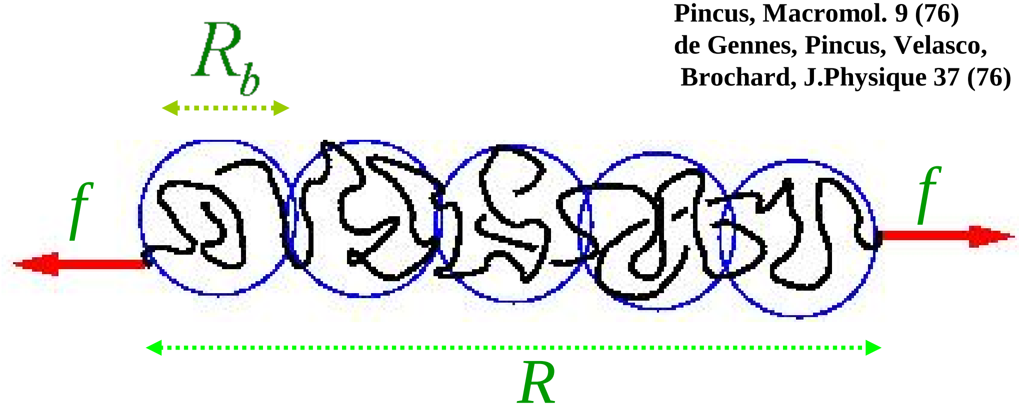
Metzler, Hanke, Dommersnes, Kantor, Kardar, PRL 88 (02)

Stretched Knots

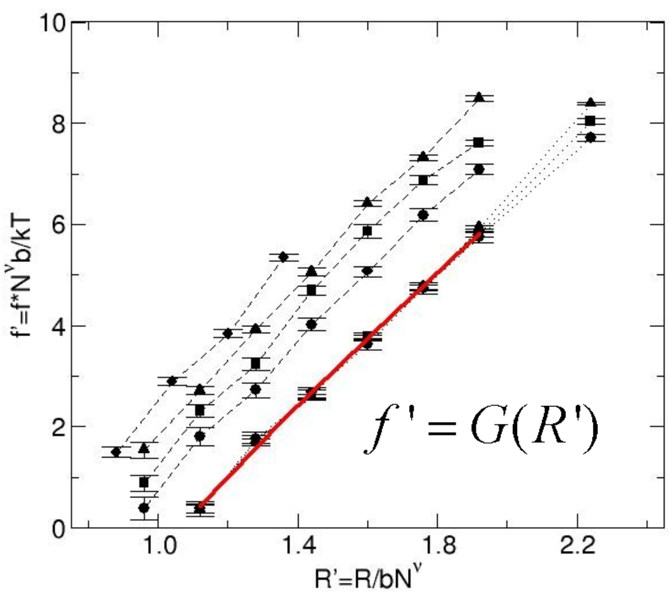


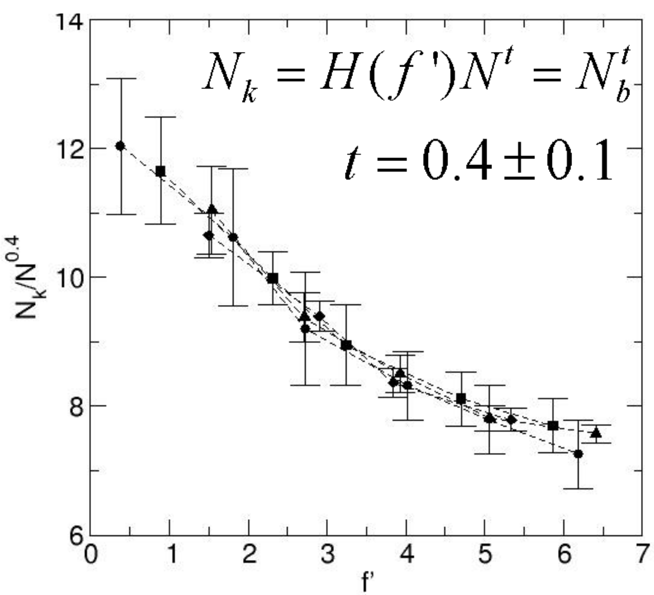
$$f' \equiv \frac{fR_g}{k_B T} \qquad R' \equiv \frac{R}{R_g} \qquad R_g = bN^{\nu}$$

Pincus, Macromol. 9 (76)
de Gennes, Pincus, Velasco, Brochard, J.Physique 37 (76)



$$N \rightarrow N - N_k$$





Farago, Kantor, Kardar EPL(2002)

Conclusions/Perspectives

- *2D knots are tight (in good solvent) and delocalize at Θ-point*
- *3D knots are sub-linear in N in good solvent*
- *Charged knots are compact*
- *Interactions between knots?*
- *Weight of knots: prime knot=1 degree of freedom?*