Star polymers and DNA in correlated environments

Viktoria Blavat'ska[•] Christian von Ferber[⊙] Yurij Holovatch[•,•]

[⊙] Applied Mathematics Research Centre, Coventry University
Jagiellonian University, Krakow & Albert-Ludwig University, Freiburg

[•] University of Leipzig

[•] Johannes Kepler University, Linz

[•] Institute for Condensed Matter Physics,
Ukranian Academy of Sciences, Lviv

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MARIE CURIE ACTIONS

Models for disordered and correlated environments

A. Weak disorder, $c_{\rm perc} < c \leq 1$

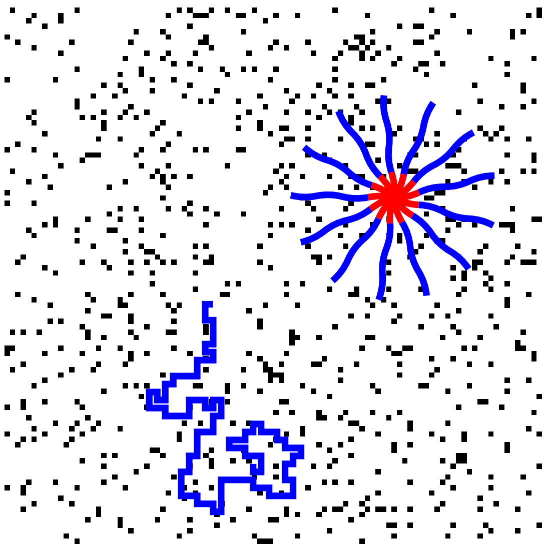
B. Strong disorder, $c = c_{\rm perc}$

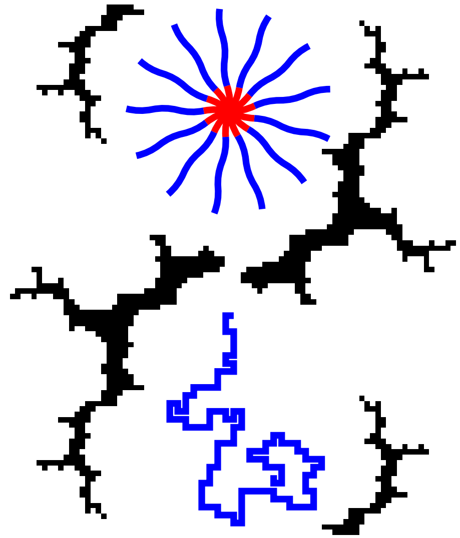
uncorrelated

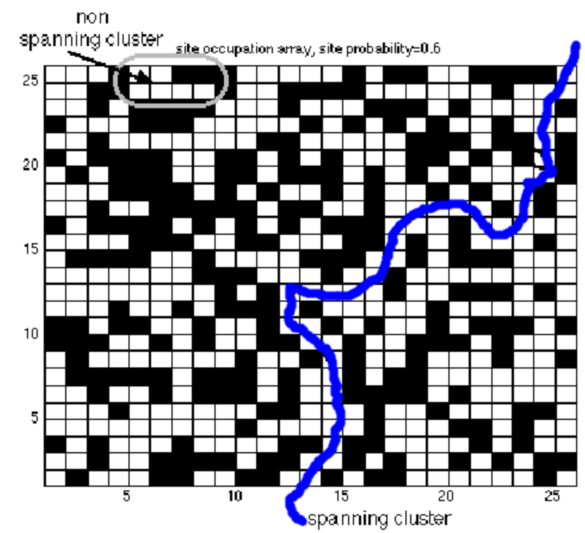
long range correlated

$g(R) \sim R^{-a}$

incipient percolation cluster







universality unchanged

$4 - d = \varepsilon$

$\nu^{\rm saw} = 1/2 + \varepsilon/16$

Kim '82

universality may change

$4 - a = \delta \leq \varepsilon/2$

$\nu = \nu^{\rm saw} = 1/2 + \varepsilon/16,$

$\varepsilon/2 \leq \delta \leq \varepsilon$: $\nu = 1/2 + \delta/8.$

Weinrib, Halperin '83

V. Blavats'ka, CvF, Yu Holovatch '01

universality and upper crit. dim. change

$6 - d = \varepsilon > 0$

$\nu = 1/2 + \varepsilon/42,$

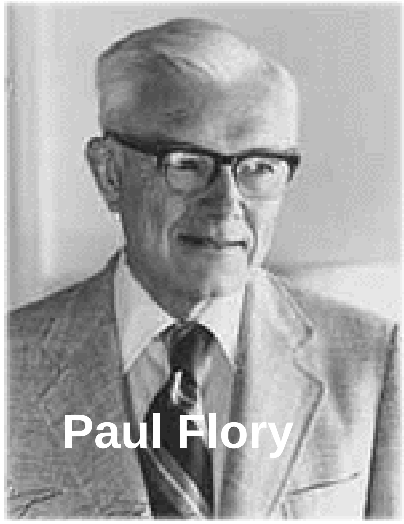
Y. Meir, A. B. Harris'89,

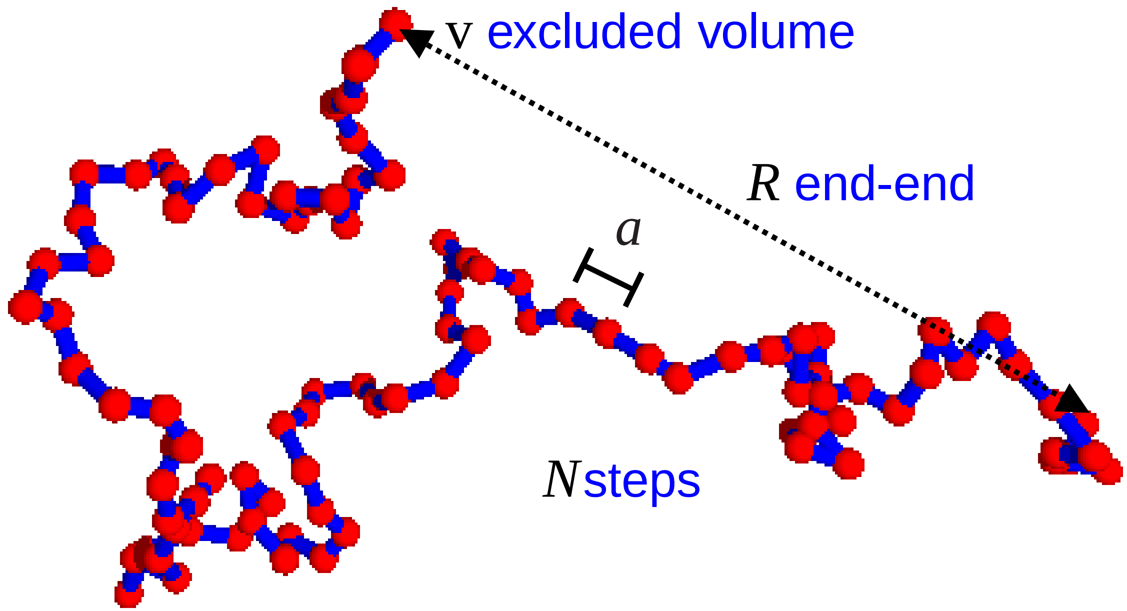
CvF, V. Blavats'ka, R. Folk, Yu Holovatch'04

O. Stenull, H.-K. Janssen '07

Polymer

self−avoiding random walk





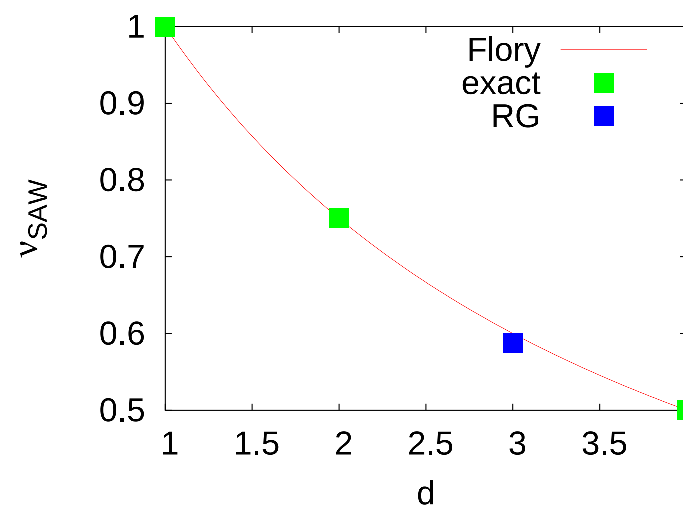
random walk $P(R) \sim e^{-\frac{R^2}{Na^2}}$

FLORY:

cloud of monomers $\rho \sim \frac{N}{R^d}$ that interact at overlap

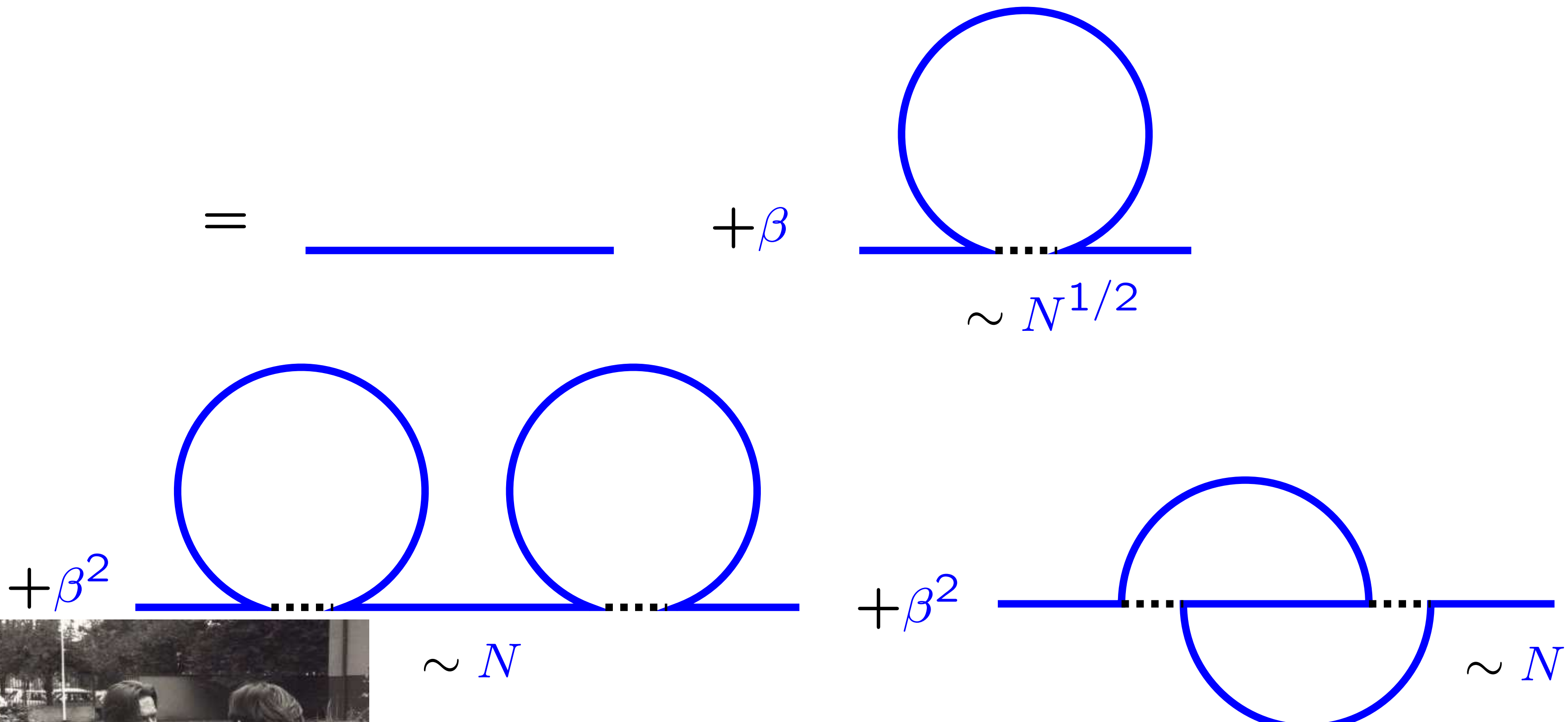
$\rightarrow$ free Energy $\frac{1}{kT}\mathcal{F}(R) \sim \underbrace{\frac{R^2}{Na^2}}_{\text{elastic}} + \underbrace{N\mathrm{v}\frac{N}{R^d}}_{\text{overlap}}$

minimize: $R \sim N^{\frac{3}{d+2}} = N^{\nu_{\text{Flory}}}$



Perturbation theory

$$\mathcal{Z}(N) = \int \prod_{j=1}^{N} \mathrm{d}r_j \exp\{-\frac{1}{4\ell^2} \sum_{j=1}^{N} (r_j - r_{j-1})^2 - \beta \ell^d \sum_{i \neq j} \delta^d(r_i - r_j)\}$$



The perturbation series diverges (in particular for $N \to \infty$).

De Gennes (1972):

Polymer theory may be mapped to spinmodel.

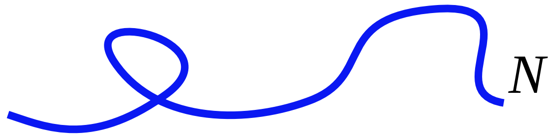
Exponents of the O(n)-symmetric spinmodel for $n = 0$

De Gennes, Phys. Lett. A 1972 (N.L. 1991)

Partition function

Number of Configurations

- linear chain



- Radius

$\langle (r_N - r_1)^2 \rangle \sim N^{\nu}$

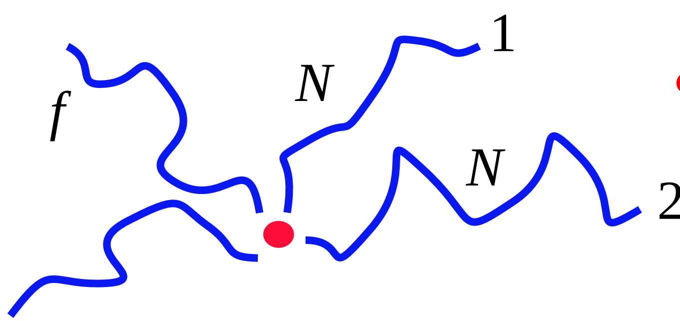
- Partition function

$Z_1(N) \sim z^N N^{\gamma - 1}$

fugacity z

- star polymer

f arms, length N

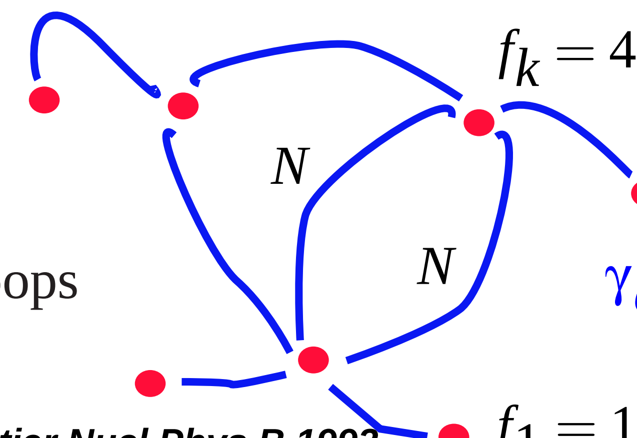


- Family of exponents γ_f

$Z_f(N) \sim z^{fN} N^{(\gamma_f - 1)}$

- network

F chains, $L_{\mathcal{G}}$ loops



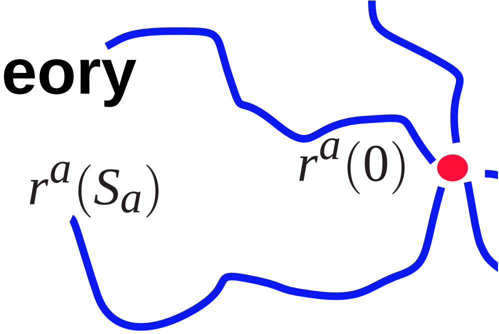
$Z_{\mathcal{G}}(N) \sim z^{FN} N^{\gamma_{\mathcal{G}} - 1}$

- linear combination

$$\gamma_{\mathcal{G}} - 1 = d\nu L_{\mathcal{G}} + \sum_k \left(\gamma_{f_k} - 1 + \frac{f_k}{2}(\gamma - 1) \right)$$

Schäfer,vF,Lehr,Duplantier Nucl.Phys.B 1992

Mapping to Lagrangean field theory



Continuous model (Edwards):

$$\frac{\mathcal{H}[r^a]}{k_B T} = \sum_a^f \int_0^{S_a} ds \left[\frac{dr^a(s)}{ds}\right]^2 + \sum_{a,b} \frac{u_{ab}}{2} \int d^d r \rho_a(r) \rho_b(r)$$

$$\rho_a(r) = \int_0^{S_a} \delta(r - r^a(s))$$

Star partition sum, chain ends at $r = 0$:

$$\mathcal{Z}_{*f}\{S_a\} = \int D[r^a] \prod_a \delta(r^a(0)) \exp\{-\frac{\mathcal{H}[r^a]}{k_B T}\}$$

local operator product "ϕ^f "

Laplace transform:

$$\widetilde{\mathcal{Z}}_{*f}\{\mu_a\} = \int_0^\infty \prod_a dS_a e^{-\mu_a S_a} \mathcal{Z}_{*f}\{S_a\} = \int D[\phi_a] \prod_a \phi_a(0) \exp\{-\frac{\mathcal{L}[\phi_a]}{k_B T}\}$$

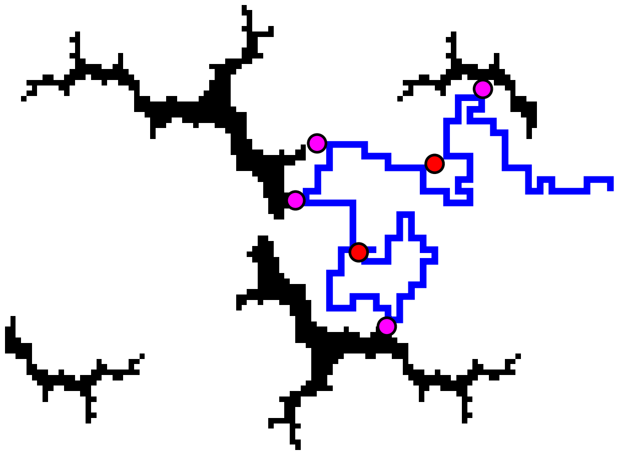
ϕ^4 – Lagrangean:

$$\frac{\mathcal{L}[\phi_a]}{k_B T} = \sum_a \int d^d r \{\frac{\mu_a}{2}\phi_a^2(r) + [\nabla \phi_a(r)]^2\} + \sum_{a,b} \frac{u_{ab}}{2} \int d^d r \phi_a^2(r) \phi_b^2(r)$$

ϕ_a is an $m = 0$ component field.

Long−range correlated medium

- self−avoidance u_0
- disorder



$$g(R) \sim R^{-a}$$

$$\widehat{g}(k) \sim v_0 + w_0 |k|^{a-d}$$

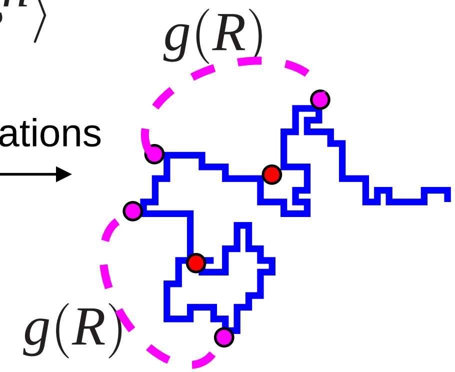
Replica

$$\langle \ln \mathcal{Z} \rangle = \lim_{n \to 0} \frac{1}{n} \langle \mathcal{Z}^n \rangle$$

average disorder configurations →

Weinrib, Halperin '83

- long−range coupling



$$\mathcal{L}_{LR} = \sum_{\alpha,\beta=1}^{n} \int \mathrm{d}^d x \mathrm{d}^d y g(|x-y|) \vec{\phi}_\alpha^2(x) \vec{\phi}_\beta^2(y)$$

n-replicated $O(m)$-symmetric m-vector $\vec{\phi}$ model

$n, m \to 0$:

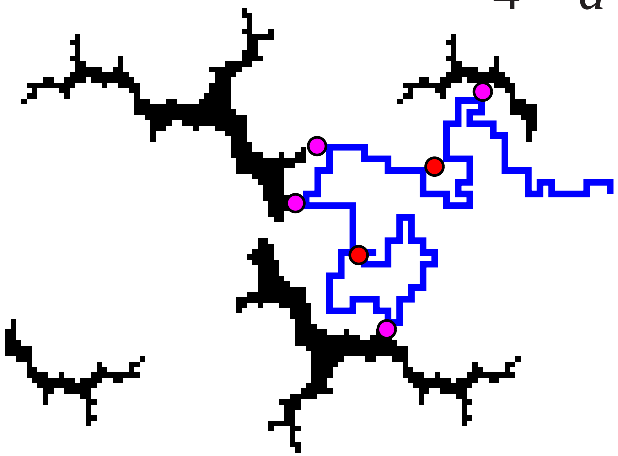
$$\mathcal{L}(\vec{\phi}) = \sum_k \sum_\alpha^n \frac{1}{2} (\mu_0^2 + k^2)(\vec{\phi}_k^\alpha)^2 + \frac{u_0}{4!} \sum_\alpha^n \sum_{\{k\}'} (\vec{\phi}_{k_1}^\alpha \vec{\phi}_{k_2}^\alpha)(\vec{\phi}_{k_3}^\alpha \vec{\phi}_{k_4}^\alpha)$$

$$+ \frac{w_0}{4!} \sum_{\alpha\beta}^n \sum_{\{k\}''} |k|^{a-d} (\vec{\phi}_{k_1}^\alpha \vec{\phi}_{k_2}^\alpha)(\vec{\phi}_{k_3}^\beta \vec{\phi}_{k_4}^\beta).$$

ε-δ expansion

● self−avoidance u_0
● disorder w_0

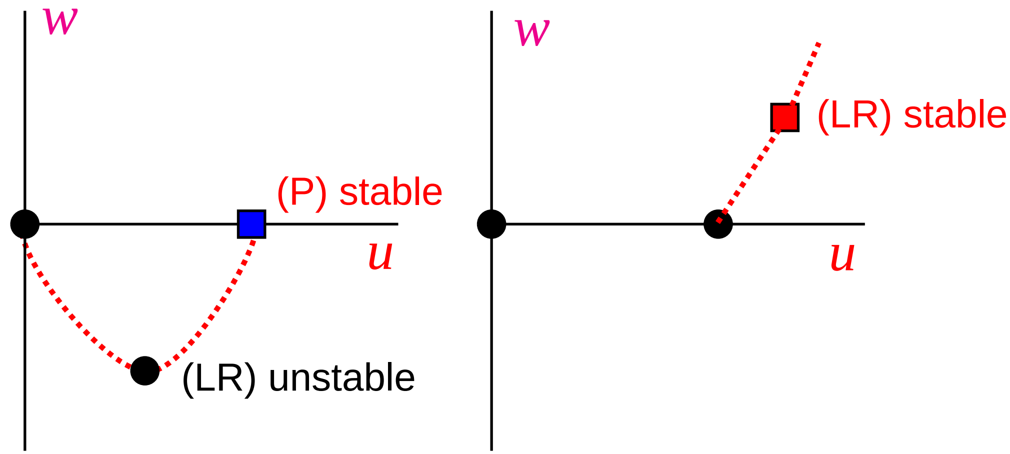
$4-d=\varepsilon$



$g(R) \sim R^{-a}$ $\quad 4-a=\delta$

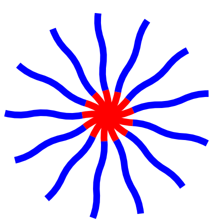
$\widehat{g}(k) \sim v_0 + w_0|k|^{a-d}$

Renormalization group flow



$\delta \leq \varepsilon/2$ $\qquad \varepsilon/2 \leq \delta \leq \varepsilon$

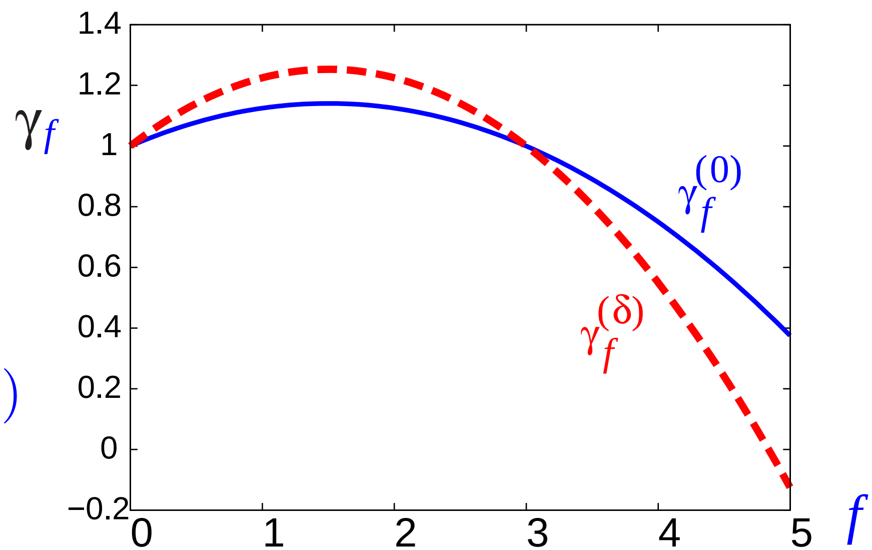
Blavat'ska, CvF, Holovatch PRE (2001)



f-arm polymer star

● Partition function

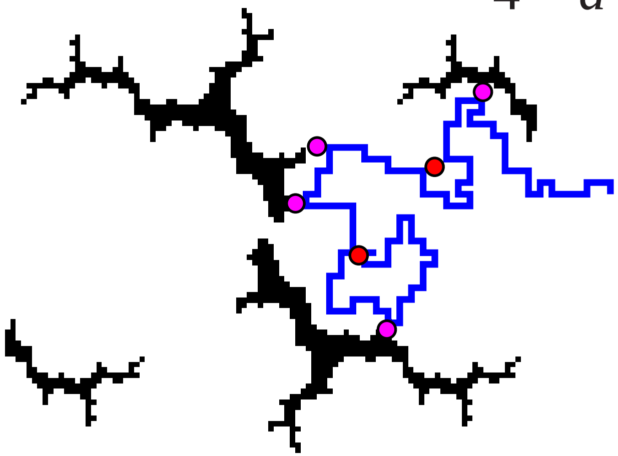
$$\mathcal{Z}_f(N) \sim z^{fN} N^{(\gamma_f - 1)}$$



Fixed d, a loop expansion

● self−avoidance u_0
● disorder w_0

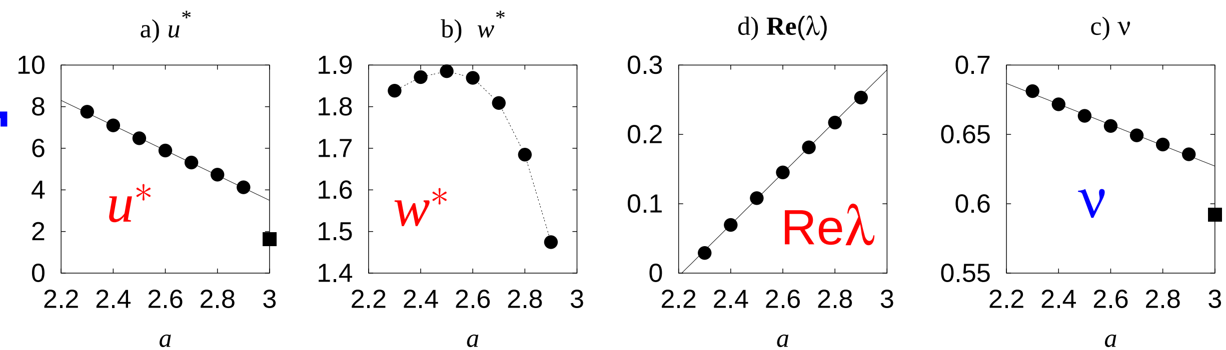
$4 - d = \varepsilon$



Renormalization group LR fixed point

Stability matrix eigenvalue λ

$R_{\text{Polymer}} \sim N^{\nu}$

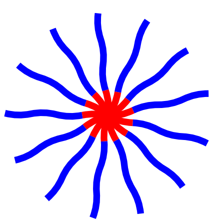


Blavat'ska, CvF, Holovatch J Phys Cond Mat (2001)

$g(R) \sim R^{-a}$

$4 - a = \delta$

$\widehat{g}(k) \sim v_0 + w_0 |k|^{a-d}$



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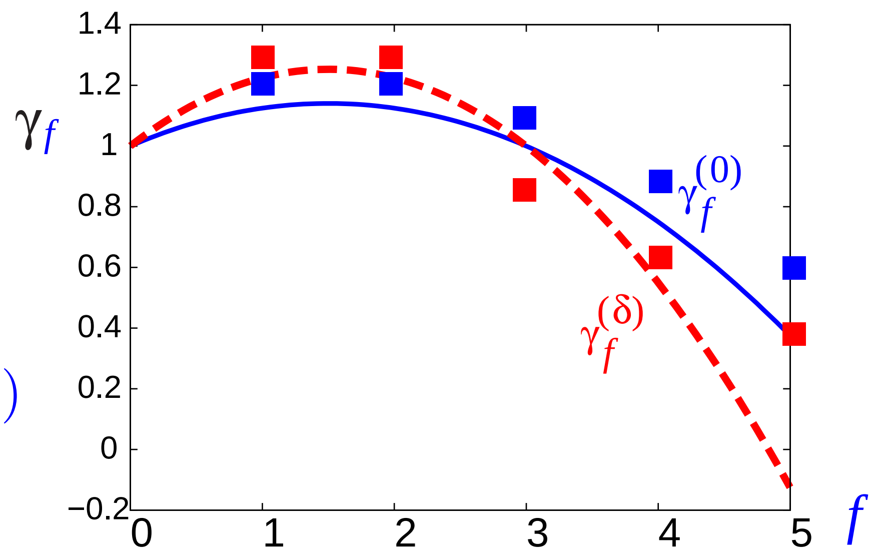
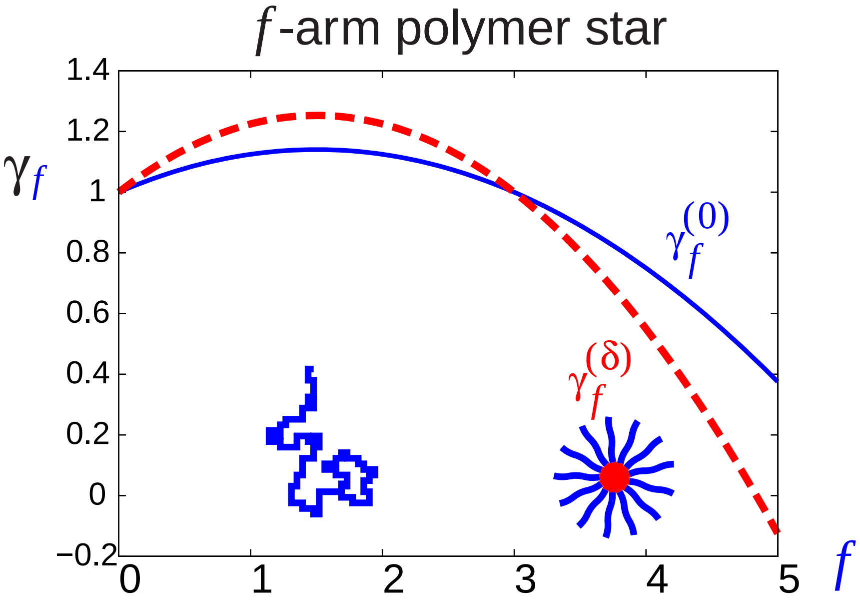


starlr12a

Static separation

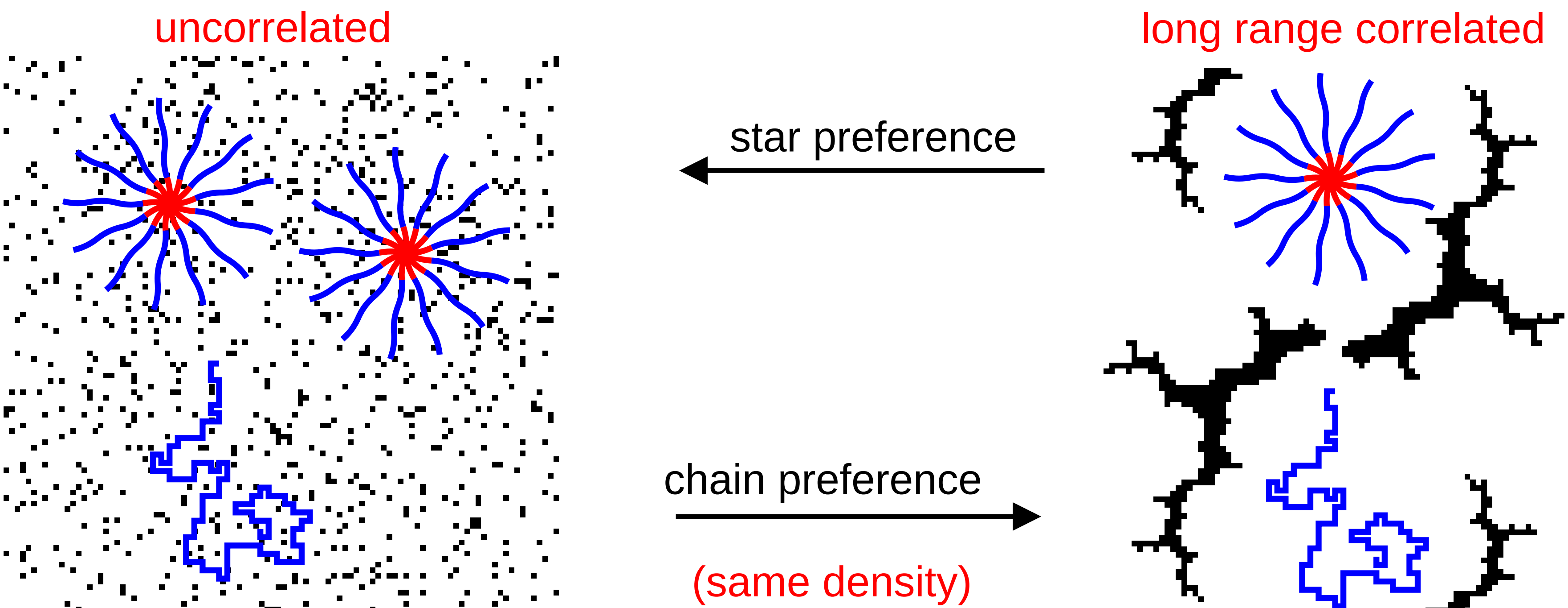


Partition function

$$Z_{*f}(N) \propto e^{\mu f N} N^{\gamma_f - 1}$$

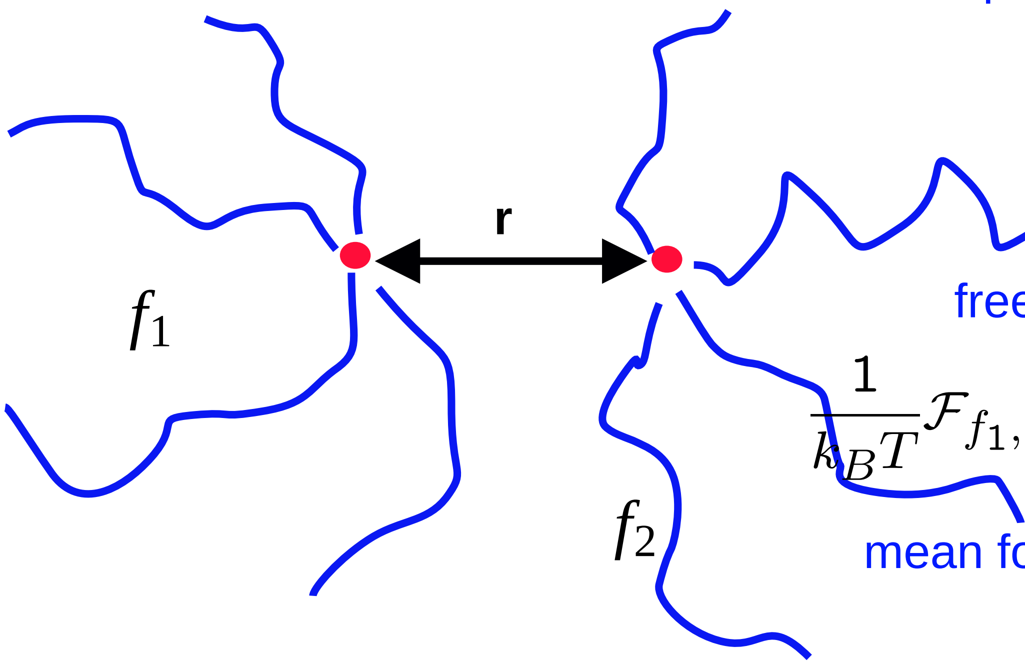
Free energy

$$\mathcal{F} = -\mu f N - (\gamma_f - 1)$$



Blavat'ska, vF, Holovatch, cond−mat (2006)

Star−star interaction



partition function:

$$\mathcal{Z}_{f_1,f_2}(r) \sim r^{\Theta_{f_1 f_2}} \mathcal{Z}_{f_1+f_2}(N)$$

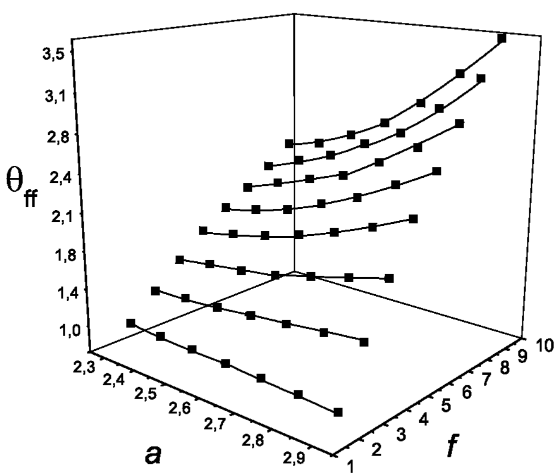
$$\nu\Theta_{f_1,f_2}(r) = \gamma_{f_1} + \gamma_{f_2} - \gamma_{f_1+f_2} - 1$$

free energy:

$$\frac{1}{k_B T}\mathcal{F}_{f_1,f_2}(r) = -\ln \mathcal{Z}_{f_1,f_2} \approx -\Theta_{f_1 f_2} \ln \frac{r}{R}$$

mean force:

$$\frac{1}{k_B T}\langle F(r)\rangle \approx \frac{\Theta_{f_1 f_2}}{r}$$



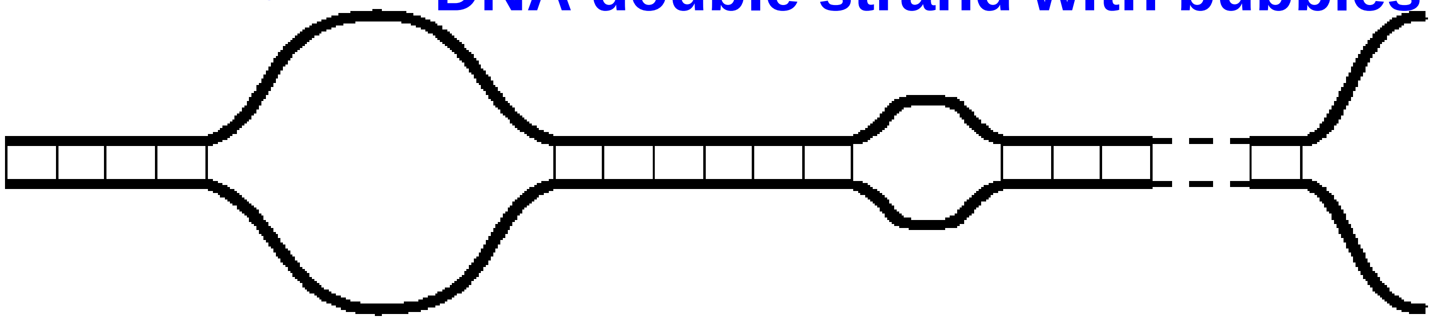
Correlated disorder weakens the effective interaction.

$\Theta_{ff}^{(a)}$ as a function of f and a at $d = 3$.

DNA denaturation

Poland, Scheraga (1966)

ℓ **DNA double strand with bubbles**



Loop size distribution $P(\ell) = \dfrac{1}{\ell^{c}}$

c determines phase transition:

$c \leq 1$:none, $1 < c \leq 2$: 2nd, $2 < c$: 1st order

Kafri,Mukamel,Peliti EPJB (2002)

Entropic contributions:

- Graph $\mathcal{G}$ $\quad Z_{\mathcal{G}}(N) \sim z^{4N} N^{-\nu\eta_{\mathcal{G}}} \qquad \eta_{\mathcal{G}} = dL_{\mathcal{G}} + \sum_k \left(\eta_{f_k} - \frac{f_k}{2}\eta_2 \right)$

- loop $\quad \ell << N: \quad Z_{\mathcal{G}}(N,\ell) \sim \left(z^{2\ell}\ell^{-c}\right)\left(z^{2N}N^{-\nu\eta_2}\right)$

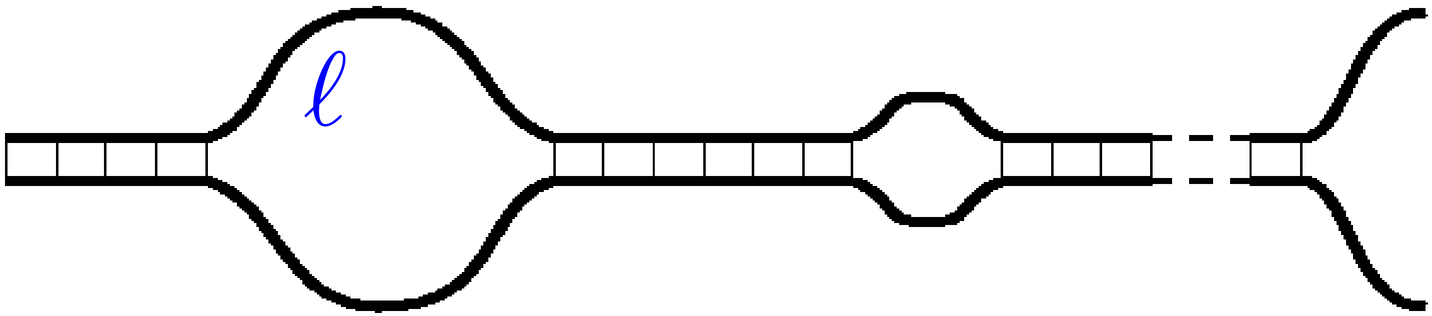
short chain expansion ***vF NucPhB (1997)***

- loop exponent

$c = \nu\eta_{\mathcal{G}} - \nu\eta_2 = d\nu + 2\nu\eta_3 - 3\nu\eta_2$ = 2.11 in 3D $\rightarrow$ 1st order transition?

DNA denaturation in correlated disorder

Poland–Scheraga model of DNA denaturation



Loop size distribution $P(\ell) = \frac{1}{\ell^c}$

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$c \leq 1$:none, $1 < c \leq 2$: 2nd, $2 < c$: 1st order

Kafri,Mukamel,Peliti EPJB (2002)

- loop exponent

$$c = d\nu - 2(\gamma_3 - 1) + 3(\gamma_1 - 1)$$

$c = 3(0.588) - 2(0.05) + 3(0.15) = 2.11$ no disorder(a=3)

$c = 3(0.68) - 2(-0.3) + 3(0.38) = 3.78$ LR disorder ($a = 2.3$)

- correlated disorder shifts the transition to 1st order.