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Renormalisation group techniques for polymers on fractal lattices

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Bridging scales: At the crossroads among renormalisation group, multi-scale modelling, and deep learning.

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Maji et al New J Phys 2010

Maji et al Phys Rev E 2014

Maji et al J Stat Mech 2017

Polymer critical behaviour

Number of polymers with N monomers: $c_N \sim \mu^N N^{\gamma-1}$ as $N \gg 1$

μ = connective constant $\rightarrow \ln \mu$ is the (asymptotic) entropy per monomer

γ = entropic exponent

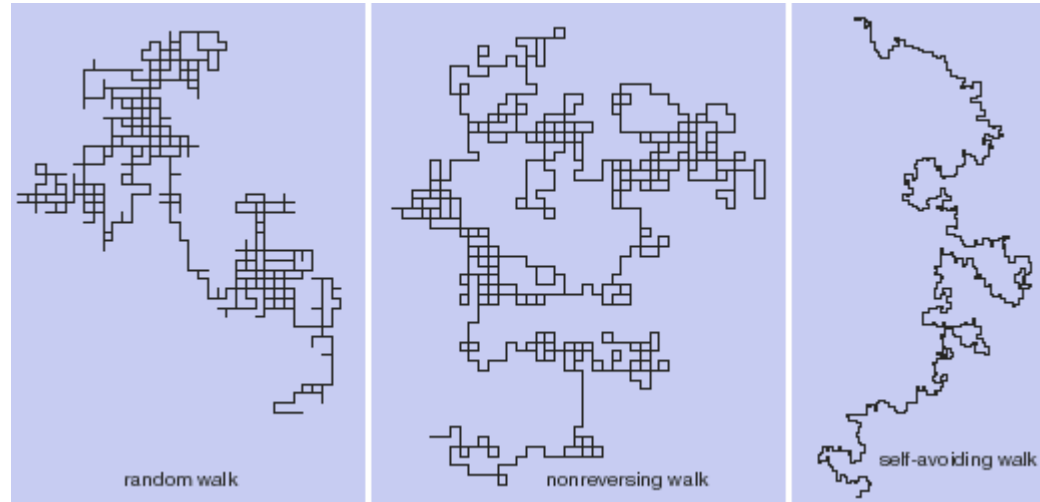
Average end-to-end distance (or gyration radius)

$R_N \sim N^\nu$ as $N \gg 1$; ν = thermal exponent

Random Walk: $\nu = 1/2$; $\gamma = 1$

(Random non interacting) Self-Avoiding Walk
($d=3$): $\nu = 0.5880(15)$; $\gamma = 1.157(3)$
SWOLLEN PHASE

[Figure from Hayes, New Scientist 1998]



SAW and O(n) spin models

Critical behaviour in the infinite N limit \leftrightarrow critical fugacity $z_c = 1/\mu$ $Z(z) = \sum_{N=1}^{\infty} c_N z^N \sim (z - z_c)^{-\gamma}$

High T-expansion of Ising model: $Z_I = \text{Tr} \prod_{\langle i, j \rangle} (1 + v s_i s_j); v = \tanh(J / \kappa_B T)$

Only graphs G consisting of L loops survive!

With n-component spins (gas of loops):

$$Z_n = \sum_G v^N n^L \quad (\text{honeycomb lattice})$$

In the $n \rightarrow 0$ limit: free energy per spin component = grand partition function for SA Polygons!

$$\lim_{n \rightarrow 0} \lim_{N_s \rightarrow \infty} \frac{1}{n N_s} \ln Z_n = \sum_{SAP} v^N$$

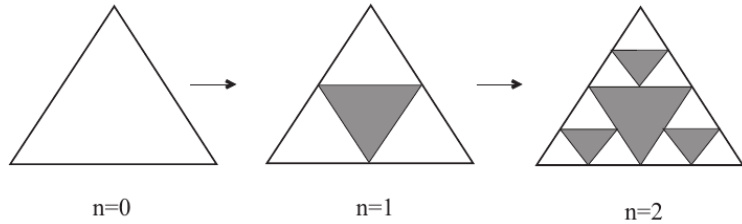
N_s = number of spins/lattice sites
 v = SAP/SAW fugacity

With the same trick: spin-spin correlation function \leftrightarrow SAW

$$G_n(k, l) = \langle \vec{s}_k \cdot \vec{s}_l \rangle; \lim_{n \rightarrow 0} \lim_{N_s \rightarrow \infty} \frac{G_n(k, l)}{n N_s} = \sum_{SAW k \rightarrow l} v^N$$

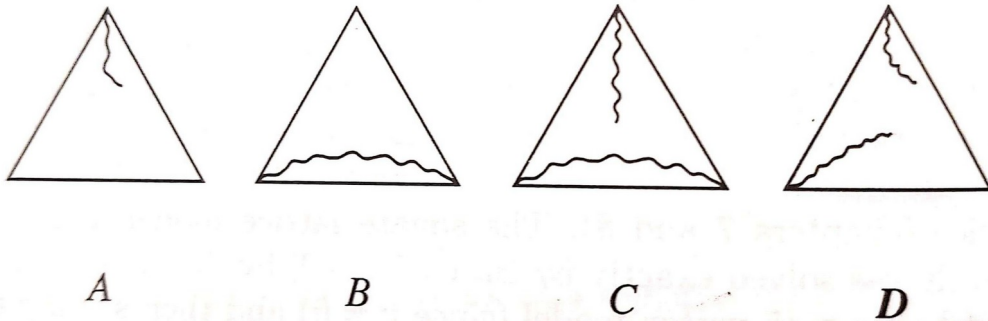
SAW on a fractal lattice

[Figure from Maji et al. NJP 2010]



Recursive construction of the Sierpinski gasket:
 $d = \ln 3 / \ln 2 \sim 1.58$

Write recursion equations for restricted partition functions (Dhar 1984)

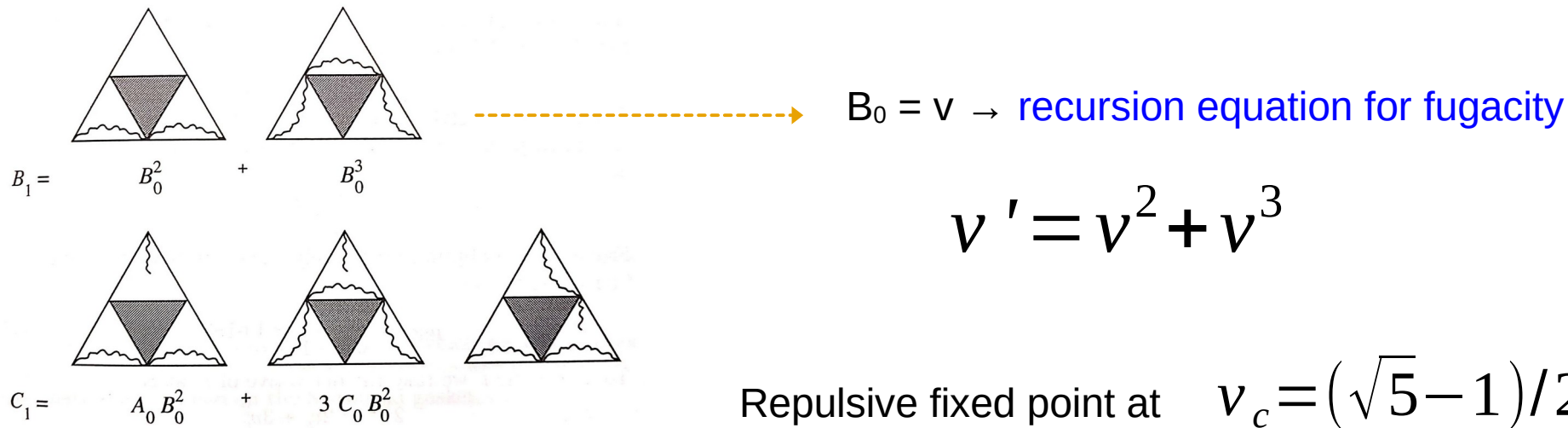


With initial conditions:

$$A_0 = \sqrt{v}; B_0 = v; C_0 = 0; D_0 = 0$$

[Figure from Vanderzande "Lattice models of polymers"]

RG technique on fractal lattice

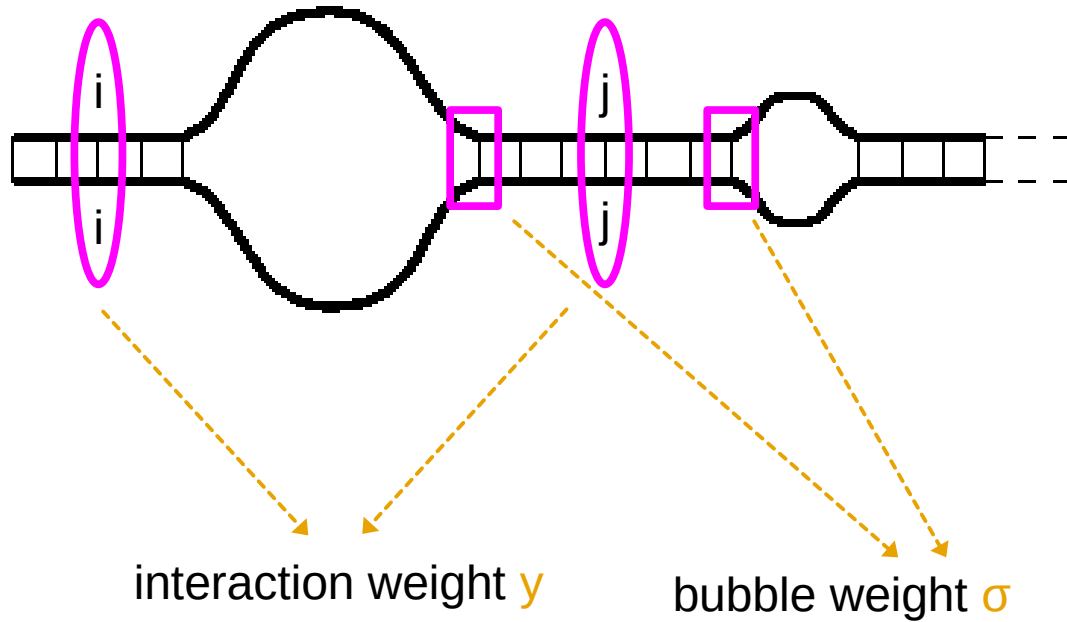


[Figure from Vanderzande "Lattice models of polymers]

Thermal exponent $\left[\frac{dv'}{dv} \right]_{v=v_c} = 2^{1/v} = 2v_c + 3v_c^2$

$v = 0.7986\dots$

A minimal model for DNA melting: Poland-Scheraga

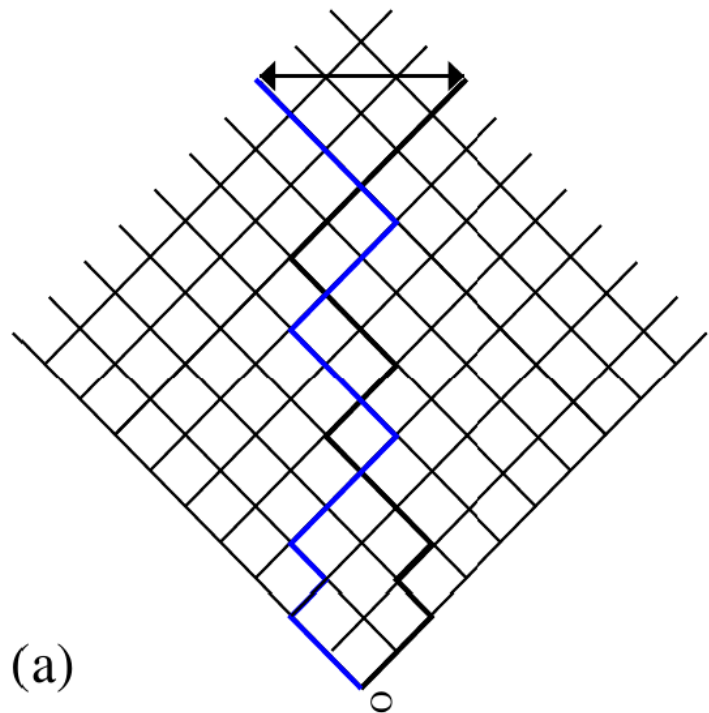


Homogeneous **ideal** polymer chains interacting with each other **only** at the same monomer index (**complementary base pairing**)

always a bound state / no melting transition in $d \leq 2$ when $\sigma = 1$ ($\sigma < 1$ or crossing constraint necessary for transition at finite T in $d \leq 2$)

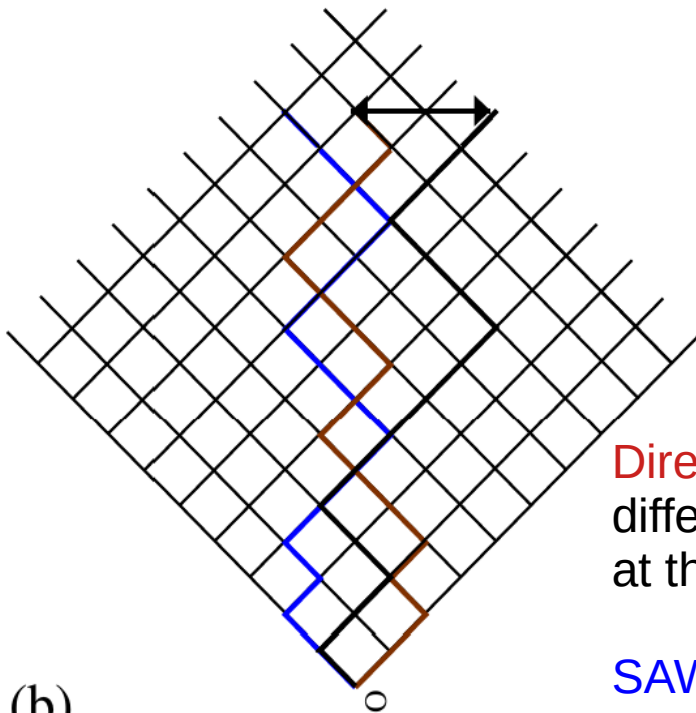
QUANTUM MAPPING monomer index \leftrightarrow imaginary time
interaction between two quantum particles with a δ -**potential**

DNA melting and bubbles in directed walk models



(a)

2 chains



(b)

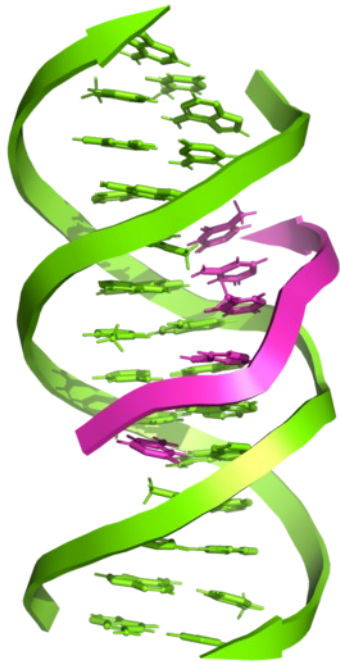
3 chains

Directedness condition →
different chains interact only
at the same monomer index

SAW in $D=d+1$ → RW in d

2 chain model exactly solvable
(with pulling force in
Marenduzzo et al. PRE 2001)

Triplex DNA



A third strand may attach to an already formed B-DNA duplex via Hoogsteen or reverse-Hoogsteen hydrogen bonds

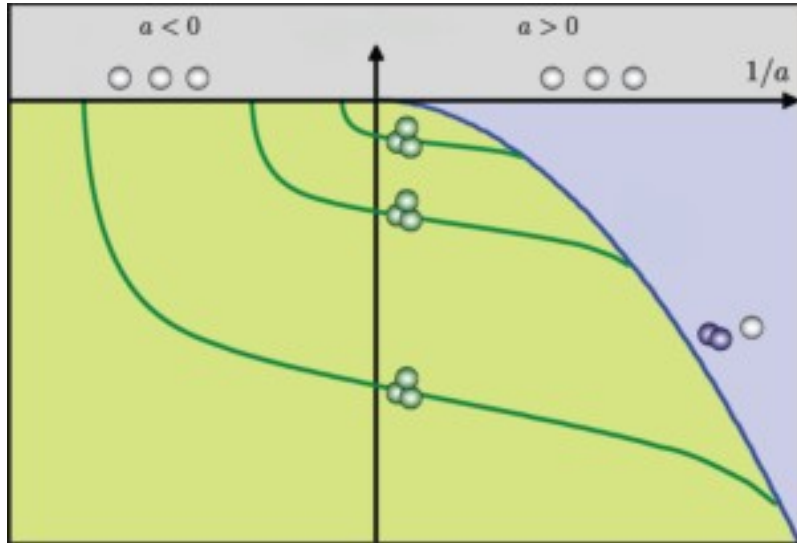
Sequence specific binding but strict base pair complementarity may be lost (always 2 Hoogsteen h-bonds per base)

Suggested/hyphotesized to regulate (inhibit) replication, transcription, protein binding to DNA

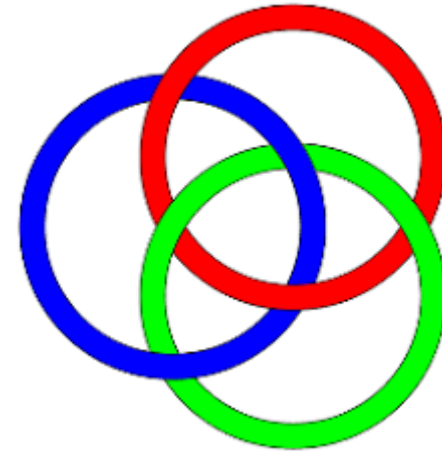
Potential therapeutic applications → delivery mechanism
([Dalla Pozza et al. Chem Rev 2022](#))

Efimov effect (from nuclear physics to cold atoms)

3 identical bosons can form a bound state when 2 cannot! → universal effect

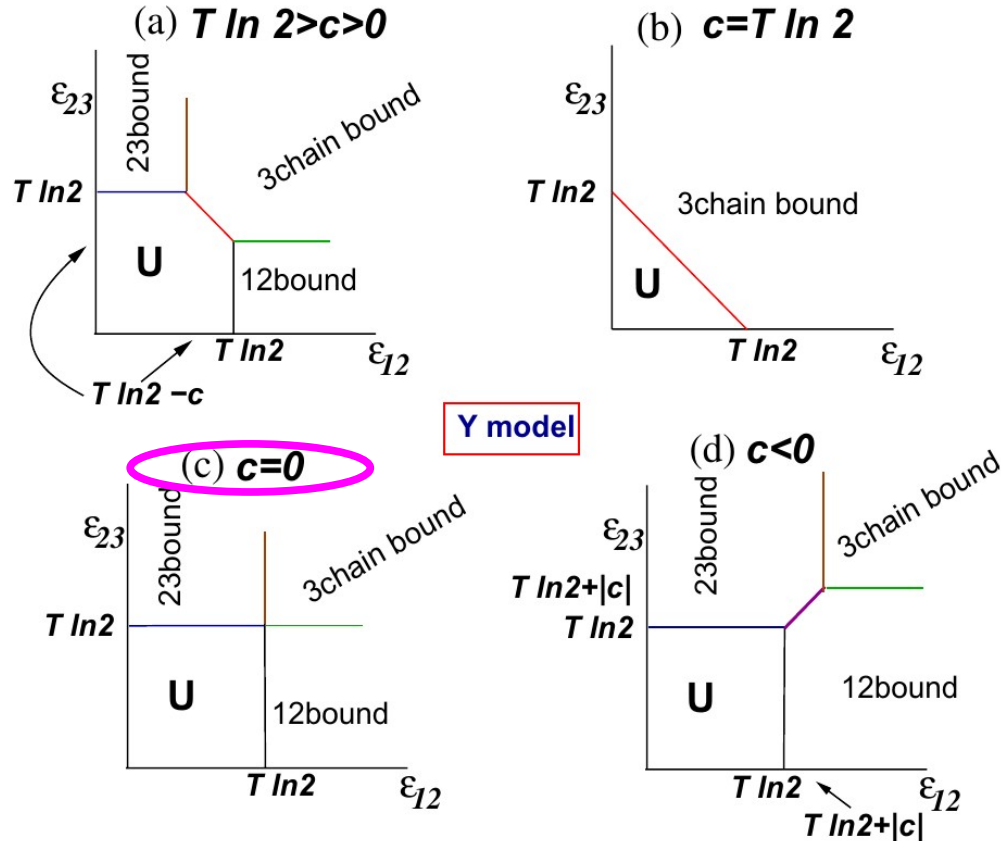


a = scattering length



“Efimov DNA”: triplex DNA stable when duplex is not?

No Efimov Dna with no bubbles



Y-fork model \rightarrow no bubbles ($\sigma = 0$)

Directed walks in $D=1+1$ (NO crossing):
2 possible steps per base

$$y = \exp(\epsilon / T); \quad c = \epsilon_{13}$$

2 chain transition at $\epsilon = T \ln 2$

same ϵ for all chains \rightarrow trivial stabilization
of 3-bound state

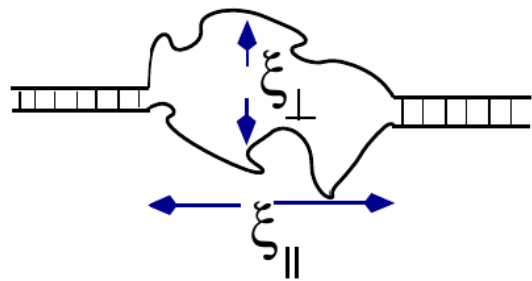
$c = 0 \rightarrow$ interactions between chains 1,3
only mediated by interactions with chain 2:
Is Efimov DNA possible with bubbles?

Efimov Dna with bubbles from scaling argument

$$\Delta F \sim -\frac{N}{\xi_{\parallel}} \mathcal{F}(R/\xi_{\perp}), \quad \varepsilon(R) \equiv \frac{\Delta F}{N} = -\frac{A}{R^z} = -\frac{A}{R^2}$$

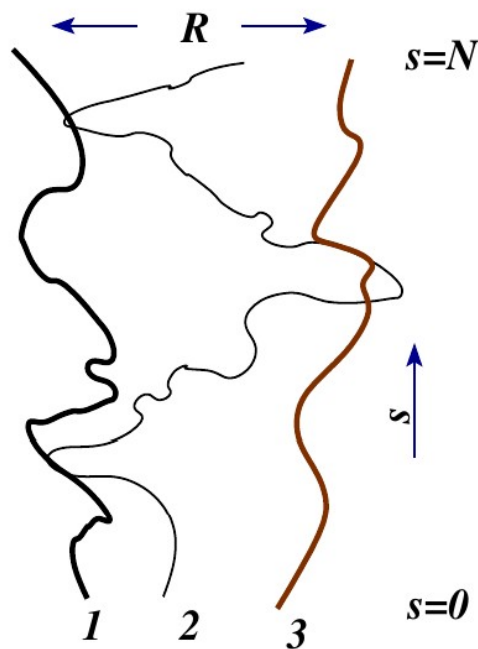
free energy change

effective universal interaction

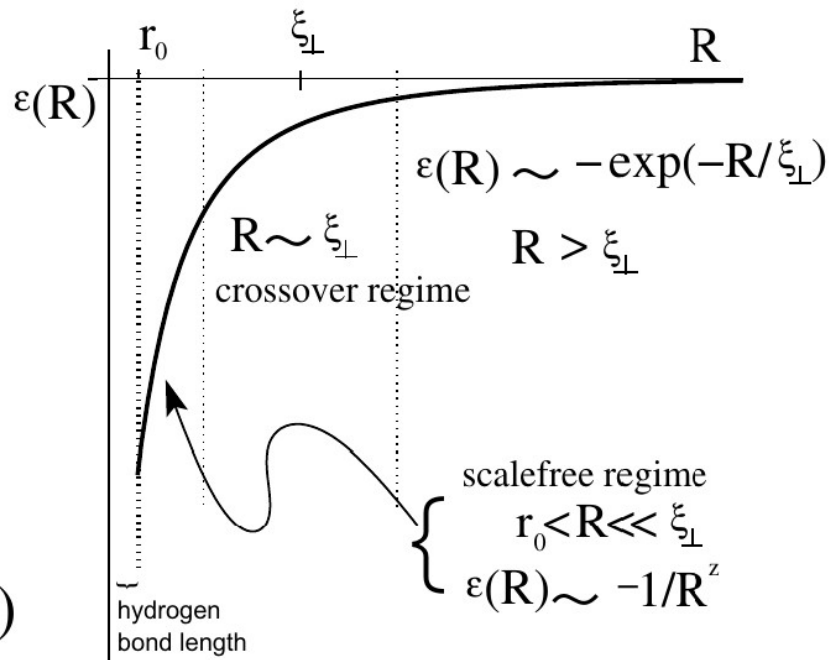


$$\xi_{\parallel} \sim \xi_{\perp}^z$$

$z = 2$ for RW



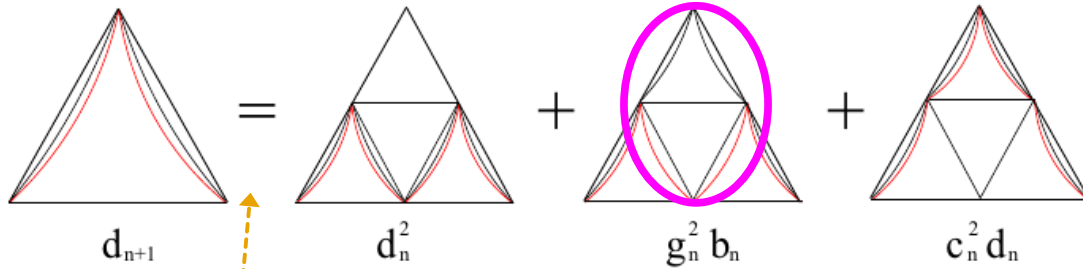
(a)



(b)

RG recursions for directed chains on Sierpinski gasket

bubbles on Sierpinski gasket



directedness constraint on Sierpinski gasket:

no horizontal steps \rightarrow different chains
Interact only at the same monomer index

$$a_{n+1} = a_n^2,$$

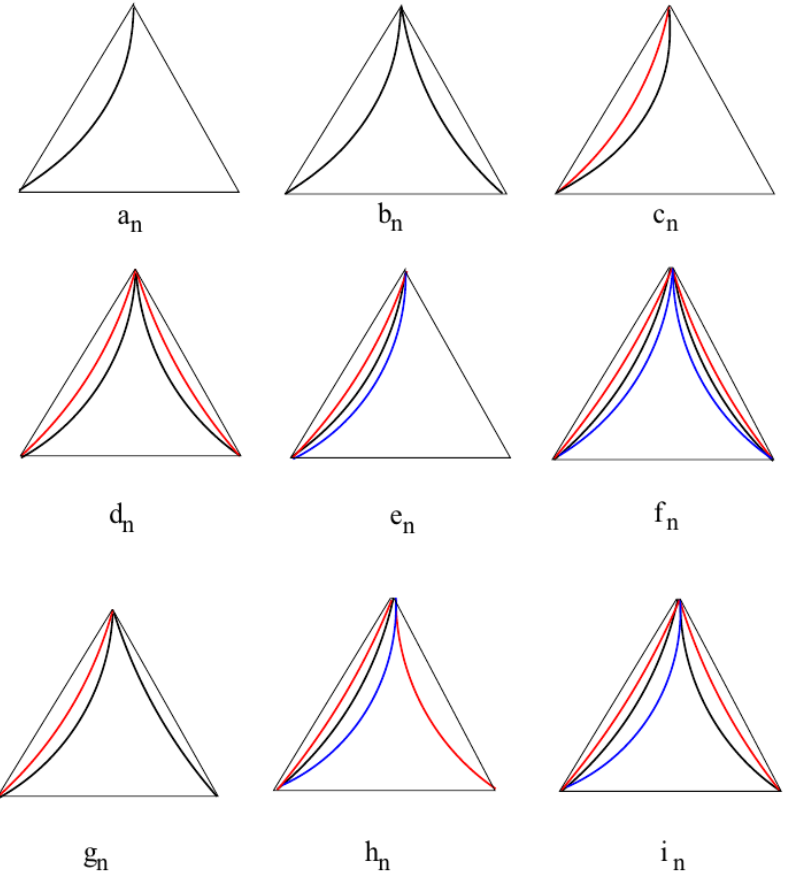
$$b_{n+1} = b_n^2 + a_n^2 b_n,$$

$$c_{n+1} = c_n^2,$$

$$d_{n+1} = d_n^2 + 2g_n^2 b_n + c_n^2 d_n,$$

$$g_{n+1} = a_n g_n (b_n + c_n).$$

recursive equations
for restricted
2 chain partition functions
(crossing allowed and $z=1$)



restricted 3 chain partition functions

RG recursions to map out the phase diagram

$$a_{n+1} = a_n^2,$$

$$b_{n+1} = b_n^2 + a_n^2 b_n,$$

$$c_{n+1} = c_n^2,$$

$$d_{n+1} = d_n^2 + g_n^2 b_n + c_n^2 d_n,$$

$$e_{n+1} = e_n^2,$$

$$f_{n+1} = f_n^2 + e_n^2 f_n + h_n^2 d_n + i_n^2 b_n,$$

$$g_{n+1} = a_n g_n (b_n + c_n),$$

$$h_{n+1} = h_n (a_n e_n + b_n c_n),$$

$$i_{n+1} = i_n (c_n e_n + d_n a_n) + g_n^2 h_n,$$

recursive equations for restricted
3 chain partition functions
(crossing not allowed and $z=1$)

with initial conditions

$$a_0 = 1, \quad b_0 = 1, \quad c_0 = y, \quad d_0 = y^2, \quad e_0 = y^2, \quad f_0 = y^4, \\ g_0 = y\sigma, \quad h_0 = y^2\sigma^2, \quad i_0 = y^3\sigma^2. \quad (10)$$

Boltzmann weights y, σ enter only through initial conditions!

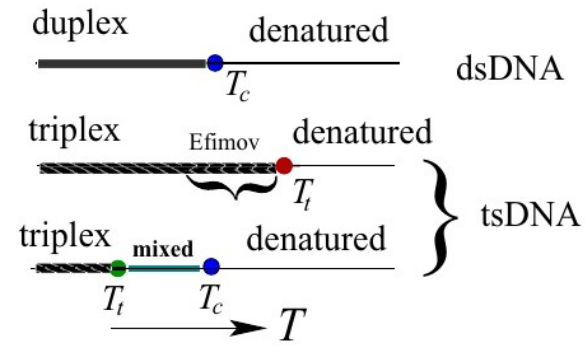
In this model $y_{12} = y_{23} = y, y_{31} = 1$

and crossing not allowed $\sigma_{ij} = \sigma, \sigma_{123} = 1$

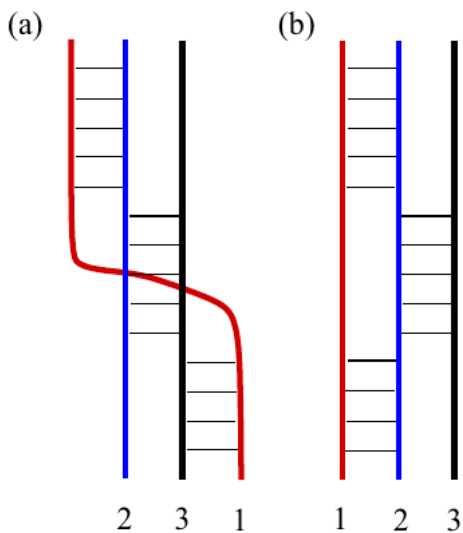
Iterate numerically and look for the leading (diverging) term

$$r_1 = \frac{\overset{\text{2-bound}}{d_{n+1}}}{\underset{\text{2 unbound}}{b_{n+1}^2}} \quad r_2 = \frac{\overset{\text{3-bound}}{f_{n+1}}}{\underset{\text{3 unbound}}{b_{n+1}^3}} \quad r_3 = \frac{\overset{\text{3-bound}}{f_{n+1}}}{\underset{\text{2b+1u}}{b_{n+1} d_{n+1}}}$$

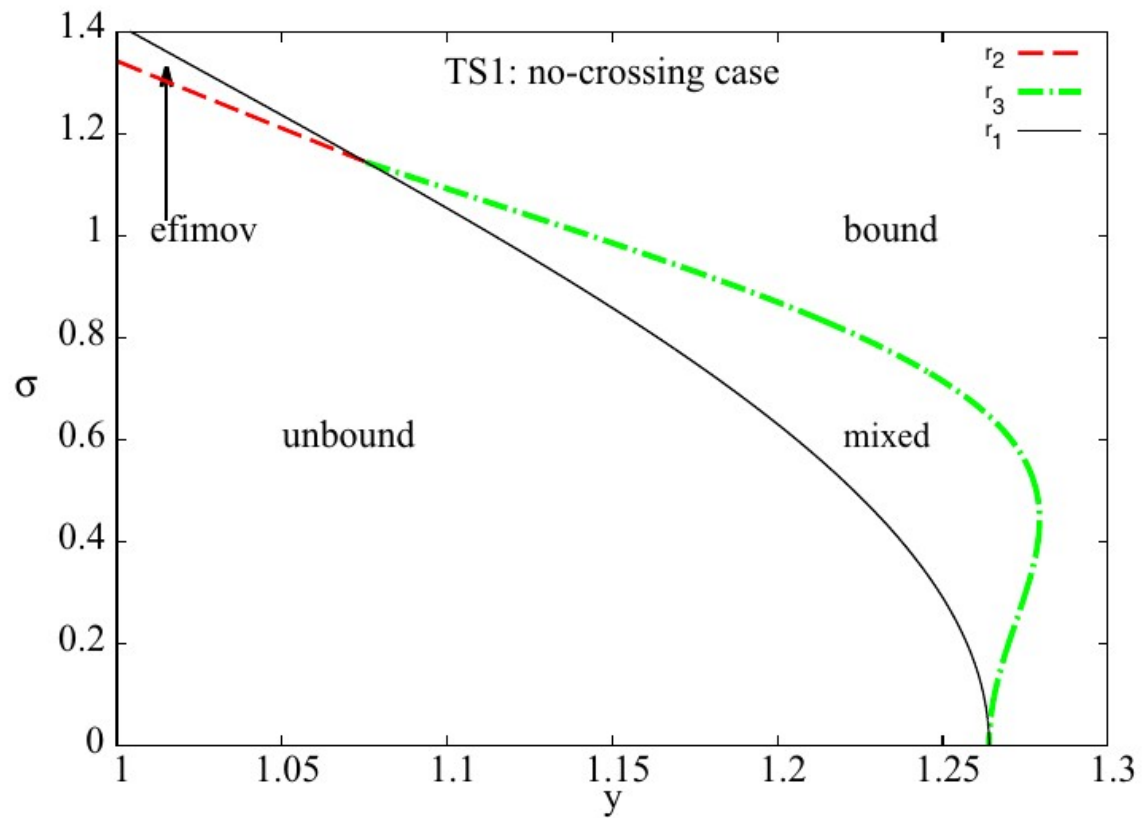
3 chain phase diagram



Possible scenarios



The mixed 2+1 phase

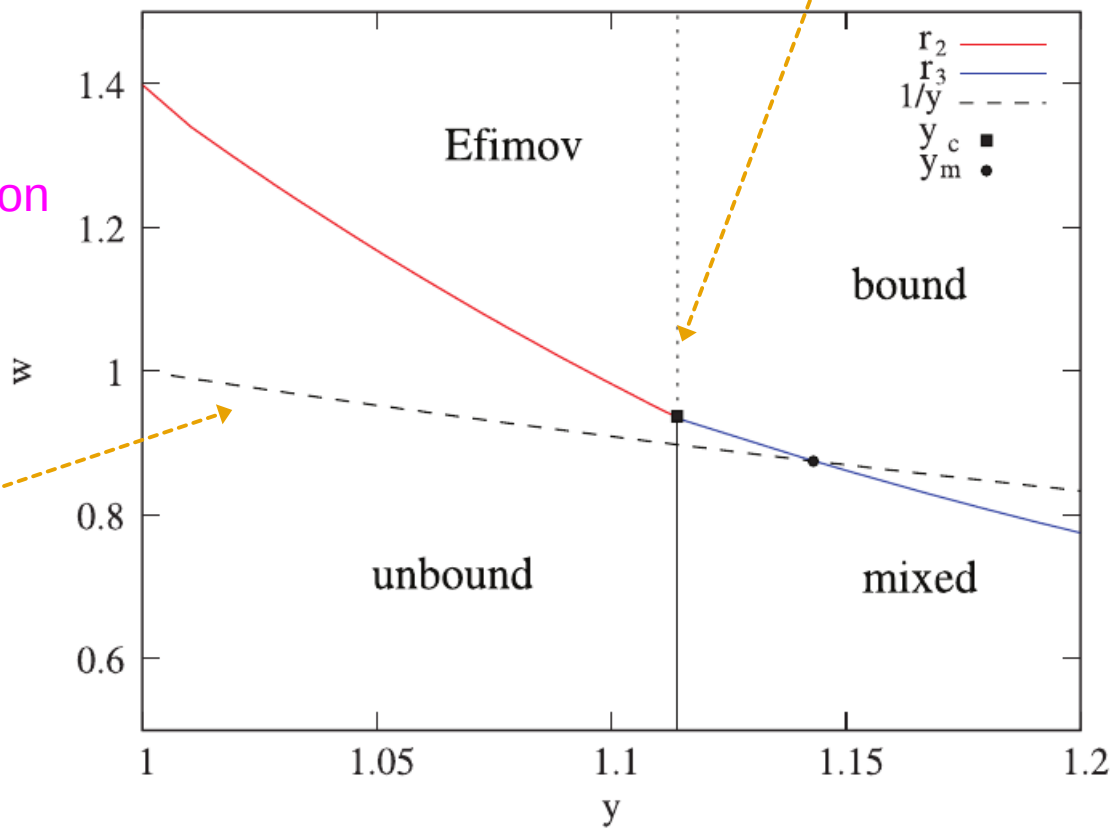


3 chain phase diagram

2 chain transition line

Same analysis with
 $w = \text{Boltzmann weight for 3-chain interaction}$
 $\sigma = 1$

$w = 1/y$ to get same results
as before with $\sigma = 1$



[Figure from Maji et al. JStatMech 2017]

Conclusions and perspectives

- real space RG is exact in fractal lattices → recursion eq. for restricted partition functions; Boltzmann weights enter through initial conditions
- phase diagram for 3 polymer chains within Poland-Scheraga model (base complementarity in DNA)
- 3 chains are bound when two are not: connection with Efimov physics (quantum mapping?) (but one should treat identical quantum particles for a full analogy)
- possibility for a mixed 2+1 phase stabilized by strand exchange: only in theory?