The polymer collapse transition in the presence of crossings

Andrea Bedini

MASCOS and Department of Mathematics and Statistics,
The University of Melbourne

ANZAMP 2nd Annual Meeting

in collaboration with A. L. Owczarek and T. Prellberg.

AUSTRALIAN RESEARCH COUNCIL
Centre of Excellence for Mathematics
and Statistics of Complex Systems

POSTERA CRESCAM LAUDE
THE UNIVERSITY OF
MELBOURNE

Outline

Outline

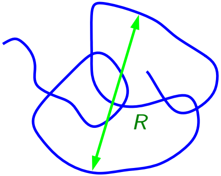
Polymers in solution

- large molecules composed of many repeated subunits
- fractals, characterised by universal exponents
- $M \propto n \simeq R^{d_f}$, d_f fractal dimension
- impenetrability gives rise to an excluded volume effect

The collapse transition

- The presence of solvent induces effective self-attraction
- A phase transition occurs as the temperature is changed

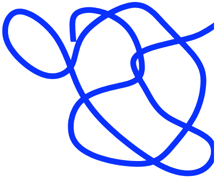
coil



$T > T_c$

d_{coil}

θ *state*



$T = T_c$

$d_{coil} < d_\theta < d_{globule}$

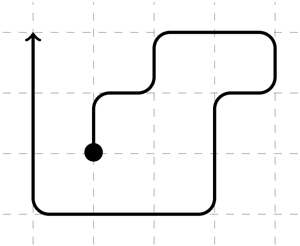
globule

$T < T_c$

$d_{globule} = d$

Self-avoiding walk

- Sequence of *distinct* vertices $x_0, x_1, \cdots, x_n$ such that each vertex is the nearest neighbour of its predecessor.



- Scaling laws

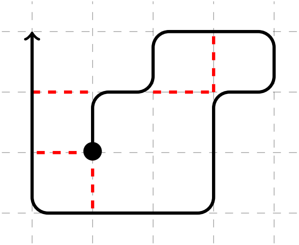
$$Z_n \simeq \mu^n n^{\gamma-1}$$

$$R_n^2 \equiv \langle |x_n - x_0|^2 \rangle \simeq A\, n^{2\nu}$$

- γ and $\nu = 1/d_f$ are universal exponent.

Interacting self-avoiding walk (ISAW)

- Introduce self-interactions (contacts m_c)



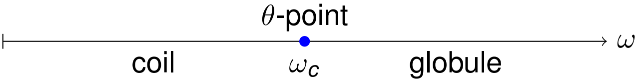
- Thermodynamics is given by

$$Z_n(\omega) = \sum_{\mathrm{SAW}_n} \omega^{m_c} \qquad f_n(\omega) = \frac{1}{n} \log Z_n(\omega)$$

$$u_n(\omega) = \frac{\partial f_n(\omega)}{\partial \omega} \qquad c_n(\omega) = \frac{\partial^2 f_n(\omega)}{\partial \omega^2}$$

Collapse transition

- As the interaction increases we reach a critical point



- Finite-size quantities are expected to obey a scaling form

$$c_n(\omega) \sim n^{\alpha\phi}\, \mathcal{C}\big((\omega - \omega_c)n^{\phi}\big)$$

where $\mathcal{C}(x)$ is a scaling function and $0 < \phi \leq 1$.

- Exponents α and ϕ satisfy the relation

$$2 - \alpha = \frac{1}{\phi}$$

Outline

Magnetic systems

- Another fundamental problem in statistical mechanics

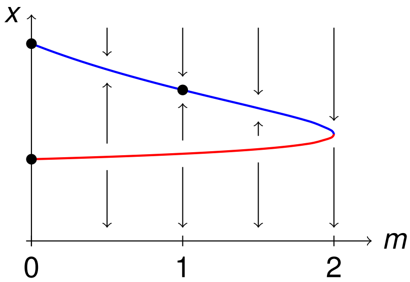
$$Z = \mathrm{Tr}\exp\left(J\sum_{\langle i,j\rangle}\vec{s}_i\cdot\vec{s}_j\right) \text{ where } \vec{s} = (s^1,\ldots,s^m)$$

- HT expansion generates polymer configurations
- Sending $m \to 0$ gives an excluded volume effect
- SAW corresponds to the critical point
- Collapse transition then corresponds to a tricritical point

Loop models

- Obtained truncating the HT expansion
- Consider an ensamble $\mathcal{C}$ of self-avoiding loops

$$Z = \sum_{\mathcal{C}} x^{length} m^{\# loops}$$



- dilute-loops branch, critical, SAW when $m = 0$
- dense-loops branch, RG attractive, globule when $m = 0$

- θ-point maps to a point on the dense branch at $m = 1$ (like the boundaries of percolation clusters)
- Also obtainable introducing vacancies at $m = 0$

Exact exponents

- Exact exponents can be obtained using Coulomb Gas techniques
- Watermelon exponents $\Delta_\ell = \Delta_\ell(m; \mathit{dilute}/\mathit{dense})$

$$\Delta_1 = 1 - \frac{\gamma}{2\nu} \qquad \Delta_2 = 2 - \frac{1}{\nu}$$

- This gives

$$\nu_{dilute} = 3/4 \quad \nu_\theta = 4/7 \quad \nu_{dense} = 1/2$$

- The transition exponents can also be computed

$$\alpha = -1/3 \quad \phi = 3/7$$

Outline

The presence of loop crossings

- This description is sensitive to the presence of crossings
- $\Delta_4 > 2$ (irrelevant) on the dilute-loop branch
- $\Delta_4 < 2$ (relevant) on the dense-loop branch
- The dense-loop branch flows to a different phase

The presence of loop crossings

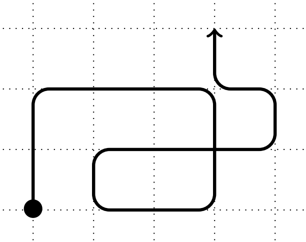
- This description is sensitive to the presence of crossings
- $\Delta_4 > 2$ (irrelevant) on the dilute-loop branch
- $\Delta_4 < 2$ (relevant) on the dense-loop branch
- The dense-loop branch flows to a different phase

- θ-point is therefore not generic
- Self-avoidance brings in an additional unwanted symmetry
- Crossings break that symmetry

What is the generic description of the polymer collapse transition?

Self-avoiding trail (SAT)

- A model for polymers with loops or polymers in thin layers.

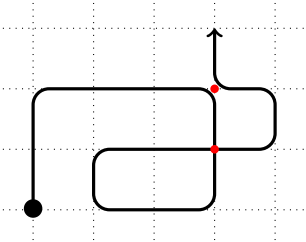


where we now require only bond-avoidance

- Free SATs are in the same universality class as SAWs

Interacting self-avoiding trails (ISAT)

- Introduce a same-site interaction on trails



- Let m_t be the number of doubly visited sites, we define

$$Z_n^{\mathrm{ISAT}}(\omega) = \sum_{\mathrm{SAT}_n} \omega^{m_t}.$$

- Energy: $u_n = \langle m_t \rangle / n$, Specific heat: $c_n = (\langle m_t^2 \rangle - \langle m_t \rangle^2)/n$

ISAT collapse transition

- As shown by Owczarek and Prellberg on the square lattice there is a collapse transition with estimated exponents

$$\phi_{\mathrm{IT}} = 0.84(3) \quad \text{and} \quad \alpha_{\mathrm{IT}} = 0.81(3)$$

- Additionally, the scaling of end-to-end distance was found to be consistent with

$$R_n^2 \simeq n\,(\log n)^2$$

- Clearly different from the θ-point
- No predictions for these exponents

$O(m)$ in the Goldstone phase

PHYSICAL REVIEW B **87**, 184204 (2013)

Loop models with crossings

Adam Nahum,[1] P. Serna,[2] A. M. Somoza,[2] and M. Ortuño[2]

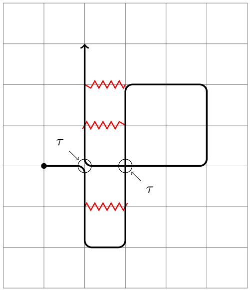
- Critical ISAT is described by the Goldstone phase of $O(m \to 1)$
- That is the generic low-temperature phase of $O(m)$
- It flows to a weak-coupling fixed point
- Dense-loops flow to this phase when crossings are allowed
- ISAT is an "infinite-order multicritical point"

Outline

The Wu-Bradley model

Competing nearest-neighbour and doubly-visited site interations

$$Z_n(\tau, \omega) = \sum_{SAT_n} \tau^{m_t} \omega^{m_c}$$



- $\tau = 0$: ISAW
- $\omega = 1$: ISAT
- $\tau = 1$: NNISAT

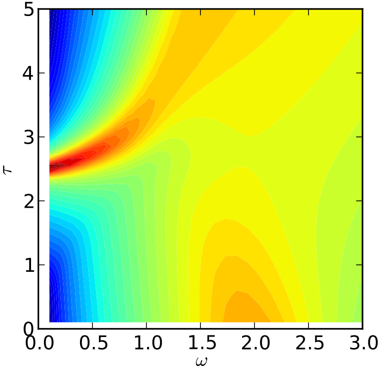
AB, A L Owczarek and T Prellberg, arXiv:1311.1034v1

Numerical phase diagram

- We sampled $\sim 10^{11}$ walks at $n = 256$ using flatPERM

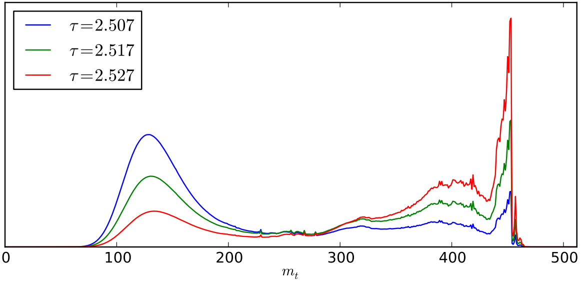
$$Z_n(\tau, \omega) = \sum_{m_t, m_c} W_{m_t, m_c} \, \tau^{m_t} \omega^{m_c}$$

- We located phase transitions by looking at the maximum eigenvalue of the matrix

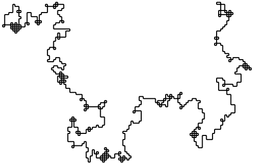


First-order transition line

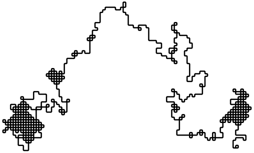
- We also simulated a vertical line with fixed $\omega = 0.5$



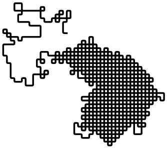
- We collected $\sim 10^{10}$ samples at $n = 1024$



$m_t = 132$

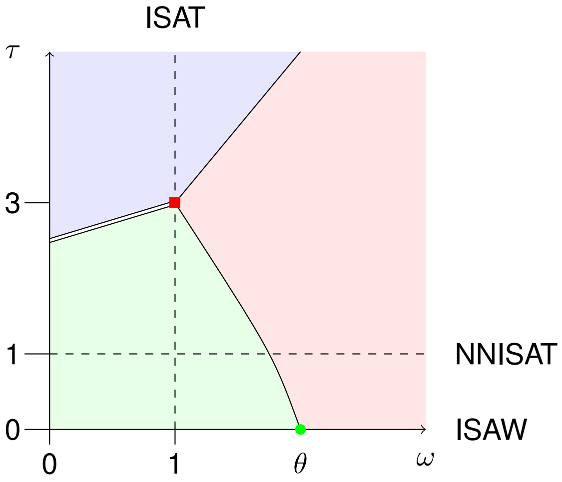


$m_t = 256$



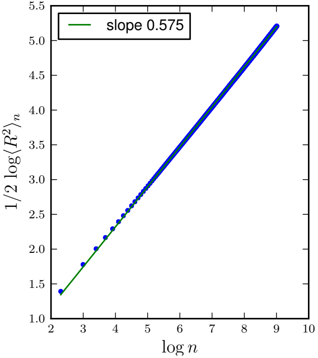
$m_t = 400$

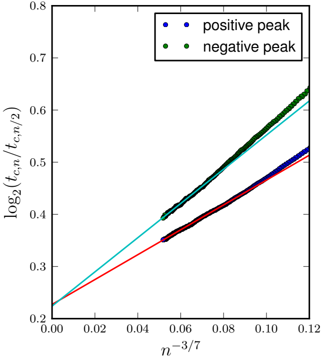
Proposed phase diagram



NNISAT exponents

Even when $\tau = 1 > 0$, we have a collapse transition with θ exponents





$\nu \simeq 0.575(5)$ vs $4/7 \simeq 0.571$ $(\alpha + 1)\phi \simeq 0.23(5)$ vs $2/7 \simeq 0.28$

Outline

Summary

- The polymer collapse problem is not fully understood yet
- A model that is fully generic is still missing
- It is not clear what universality class INNSAT is

Summary

- The polymer collapse problem is not fully understood yet
- A model that is fully generic is still missing
- It is not clear what universality class INNSAT is

Thanks