A tale of two napkins: Interacting Partially Directed Walks

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Outline			
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Talk outline



Some Physics involved in polymers (Motivation)

- 2 Mathematical Preliminaries
- Partially directed walks
- Interacting Partially directed walks
- 5 Variable flexible Interacting Partially directed walks

Outline

Polymers/Motivation

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Modelling of Polymers in Solution

- Polymers: long chains of monomers
- "Coarse-Graining": beads on a chain
- "Excluded Volume": minimal distance between beads
- Contact with solvent: effective short-range interaction
- Good/bad solvent: repelling/attracting interaction



Outline

Polymers/Motivation

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Modelling of Polymers in Solution

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A Model of a Polymer in Solution

Random Walk + Excluded Volume + Short Range Attraction

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A Polymer Phase Transition: Collapse (θ -point)

- Polymers are often 'Fractal': length n, spatial extension $R \sim n^{\nu}$ and the mass $m \propto n \sim R^{d_{fractal}}$ giving $\nu = 1/d_{fractal}$.
- A "Phase transition" occurs as temperature is changed: Polymer Collapse, aka Coil-Globule Transition, aka Θ-Point



 $T > T_c$: good solvent swollen phase (coil): $d_{fractal} < d$



 $T = T_c$: Θ -polymer: $d_{fractal} \approx 2$

 $T < T_c$: poor solvent — collapsed phase (liquid-like globule): $d_{fractal} = d$

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The Canonical Polymer Lattice Model

- Polymer → self-avoiding random walk (SAW)
- Physical space \rightarrow regular lattice eg \mathbb{Z}^3 or \mathbb{Z}^2
- Sites beads monomers



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The Canonical Polymer Lattice Model

- Polymer \rightarrow self-avoiding random walk (SAW)
- Physical space \rightarrow regular lattice eg \mathbb{Z}^3 or \mathbb{Z}^2
- Sites beads monomers



- Introduced by Orr in 1947
- Still no closed form solution for the number of walks of length n
- Can consider limit n → ∞ as a critical phenomenon (de Gennes) (as well as a phase transition in the thermodynamic limit as temperature is varied).

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The Canonical Collapsing Polymer Lattice Model

Interacting Self-Avoiding Walk (ISAW)

- Start with a SAW and add 'interactions'
- Quality of solvent \rightarrow short-range interaction energy -J
- Interactions are between (non-consecutive) nearest neighbours



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Variations and extensions

- ISAW even more difficult mathematically
- From work of de Gennes and later by Duplantier and Saleur expect "Tricritical" collapse transition
 - The $n \to \infty$ critical phenomena changes from second order at high temperatures to first order-like at low ones.
 - Thermodynamic limit phase transition is second order
- $\bullet\,$ At low temperatures sometimes can expect $\beta\text{-sheet}$ structures: long folds
- Studies of effects of other forces and physical effects
 - Surface phenomena: polymer adsorption
 - Stiffness: rod-to-coil transition
 - Stretching polymers: micromanipulation experiments
- Search for exactly solvable model ... Start on the square lattice

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Generating functions versus partition functions

Partition function

 $Z_n(\text{parameters}) = \sum_{\text{walks of length } n} Boltzmann weight of configuration depending on parameters}$

and

Boltzmann weight =
$$e^{-\text{Energy of configuration}/k_BT}$$
 eg. $\omega = e^{J/k_BT}$

where T is the temperature ($\beta = 1/k_BT$), while the generating function is

$$G(\mathbf{z}; \text{parameters}) = \sum_{n \ge 0} Z_n(\text{parameters}) \, \mathbf{z}^n$$

However, often we evaluate a generating function in terms of composite variables such as

x = pz

where p is a parameter. This comes about as a natural consequence of the method.

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Generating functions versus partition functions II

The setup

Let our parameters be $p_j = e^{\beta \epsilon_j}$ where $-\epsilon_j$ is the energy associated with some countable feature of our walk. Let there be $m_j(\varphi_n)$ occurences of this feature in walk configuration φ_n of length n. Then the partition function

$$Z_n(p_1, p_2, \ldots) = \sum_{\varphi_n} \prod_j p_j^{m_j(\varphi)}$$

and we define a reduced free energy as

$$\kappa(p_1, p_2, \ldots) = \lim_{n \to \infty} \frac{1}{n} \log Z_n(p_1, p_2, \ldots)$$

Assuming this limit exists the radius of convergence $z_c(p_1, p_2, ...)$ of the generating function $G(z; p_1, p_2, ...)$ is related to the free energy as

$$\kappa(p_1,p_2,\ldots)=-\log z_c(p_1,p_2,\ldots)$$

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Phas	e transition			

- Critical phenonemon at $n \to \infty$
- "Thermal" phase transition as parameters are varied
- Thermal phase transition implies non-analyticity in free energy and hence z_c as a function of the parameters.
- We expect a collapse phase transition as ω is varied at $\omega = \omega_t = e^{J/k_b T_t}$

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Some Exponents

• Generically we expect that for $T \ge T_t$, where T_t is the tricritical collapse θ -temperature

$$Z_n \sim A e^{\kappa n} n^{\gamma-1}$$

which implies

$$G(z) \sim rac{A'}{(z-z_c)^{\gamma}}$$

- $\bullet\,$ Have already met the size exponent $\nu\,$
- Near the collapse transition we expect

$$\kappa \sim C |T - T_t|^{2-\alpha}$$

This introduces the thermal exponent α .

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Some More Exponents

• As we have just introduced, near the collapse transition we expect

$$\kappa \sim C |T - T_t|^{2-lpha}$$

- Due to the relationship between the free energy and the radius of convergence of the generating function the shape of the curve z_c(T) is related to α.
- The exponent relating the n→∞ critical phenomena and the thermal phase transition of collapse is the so-called *crossover* exponent φ. Eg.

$$R \sim n^{
u_t} \mathcal{R}((T - T_t)n^{\phi})$$

where \mathcal{R} is a *scaling* function.

It can be seen that

$$\phi = 1/(2-\alpha)$$

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Partially directed walks: the beginning

- Soon after Orr's introduction of SAW workers defined restricted sets of SAW so as to analyse SAW (Frisch, Collins and Friedman, 1951)
- Fisher and Sykes (1959) considered partially directed walk configurations so as to provide bounds on SAW numbers
- Temperley (1956) had already considered them as models of magnetic model phase boundaries
- A flurry of activity occurred in the 1980's with Szpilka, Privman, Svrakic, Forgas and Frisch (yes the same one) considering generalisations and adding various parameters

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What is a partially directed walk?



Starting at the origin allow only steps in the (1,0) (East), (0,1) (North) and (0,-1) (South) directions

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No parameters: our first model



• The generating function is *rational* with a simple pole ($\gamma = 1$) at $z_c = \sqrt{2} - 1$.

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Our first Singularity diagram



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Properties of a partially directed walk



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Properties of a partially directed walk

$$s_x = n_x \sim n^{\nu_{\parallel}}$$

$$s_y \sim n^{
u_\perp}$$

 $\langle |r| \rangle \sim n_r^{\nu}$

These have been found as $\nu_{\parallel}=1,\,\nu_{\perp}=1/2$ and $\nu_r=0$

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Counting vertical and horizontal steps separately



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Counting vertical and horizontal steps separately

The generating stays rational

$$G(x,y) = \frac{1+y}{1-y-x-xy}$$

Reinterpreting with a force parameter $h = e^{\beta f_x}$ gives

$$G(z;h)=\frac{1+z}{1-z-hz-hz^2}.$$

which has a simple pole at $\frac{z_c}{2h}(h) = \frac{\sqrt{h^2+6h+1}-1-h}{2h}$.

This is an analytic function of h > 0 so no finite force produces a phase transition.

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Rod to coil Transition



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Counting vertical and horizontal steps separately

• Privman and Frisch (1988) found the generating function and again it stays rational.

Once again $z_c(b)$ is analytic function of b > 0 so no finite bend energy produces a phase transition. The rod-to-coil "phase transition" is a zero temperature effect. Outline

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Interacting partially directed walks

Interacting partially directed walk of n = 21 steps including m = 6 nearest neighbour contacts nearest-neighbour "contact" Generating function weight $\omega^6 z^{21}$ ∞ Boltzmann weight ω^6 where $\omega = e^{\beta J}$ (nearest neighbour energy -J)

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IPDW history

The psychedelic era

- In 1968 and 1970 Zwanzig and Lauritzen considered a more restricted set of walks (partially directed walks that must change vertical direction after each horizontal step).
- They found a collapse transition.
- Their work went essentially unnoticed by the workers on self-avoiding walks.

The Thatcher Years

- During the 80's there was lots of work on magnetic/liquid phase boundaries including so-called Solid-on-solid models (aka Partially directed walks in 2 dimensions)
- Also work on related polymer adsorption transition in late 80s/early 90s

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IPDW history

- In 1989 one generalisations of the adsorption problem was considered by Veal, Yeomans (Oxford) and Jug.
- They considered partially directed walks above a sticky wall but also with nearest neighbour attraction.
- They numerically analysed the transfer matrices and found an accurate value of the tricritical point without any surface attraction at

 $(\omega, z) = (3.382976, 0.2955977)$

- ALO moves to Oxford and becomes interested in interfacial phenomena like depinning and wetting transitions
- One thing leads another and IPDW is considered

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Solution on the special curve $z = 1/\omega$

Binder, Owczarek, Veal and Yeomans (1990) used the transfer matrix method to examine the model along the curve

$$z = 1/\omega$$

They found a singular point at the solution of a cubic giving

$$\omega_t^{-1} = \frac{1}{9} \left[(17 + 3\sqrt{33})^{1/3} + (17 - 3\sqrt{33})^{1/3} - 1 \right]^2 = 3.3829757 \dots$$

They argued on physical grounds that this must be the tricritical point. Further that for $\omega > \omega_t$ one has $z_c(\omega) = 1/\omega$.

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IPDW history

• Using generating function methods one can easily find that

$$1 + G(z; \omega = 1/z) = \sqrt{\frac{1-z}{1-3z-z^2-z^3}}$$

- For $\omega > 3.382976...$ the generating function is finite
- Along this curve the singularity at (3.382976..., 0.2955977...) is algebraic: a divergent square root singularity to be precise.
- We define

$$\gamma_t^{\rm tangential} = 1/2$$

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Singularity diagram 2



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The other side of the world

- Whittington (Toronto) and Guttmann (Melbourne) continue their quests for solution of SAW problems
- Brak moves from Oxford to Melbourne and becomes interested in SAWs and Polymers
- Brak, Guttmann and Whittington investigate IPDW

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Temperley method

Now Brak and Guttmann had uncovered the method used by Temperley in 1956

- Consider the generating function for walks with last vertical segment of length *r*
- Find a recurrence for these by adding an extra column of walk
- Use a *q*-series Ansatz

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Solution

Let us define the variable

$$q = \omega z$$

so the special curve becomes q = 1. Solving the recurrence gives

$$1+G(z;\omega)=\frac{z^2(z-1)g_0^{(1)}}{z^2(1+\omega+z-\omega z)g_0^{(1)}-2zg_1^{(1)}}.$$

where

$$g_r^{(1)} = z^r + z^r \sum_{m=1}^{\infty} \frac{(z-q)^m q^{m(m+1)/2}}{\prod_{k=1}^m (q^k - \omega) \prod_{k=1}^m (q^k - 1)} q^{mr}.$$

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- The functions involved were later indentifies as *q*-Bessel functions.
- Each $g_r^{(1)}$ converges for any q < 1
- So the singularities of $G(z; \omega)$ may be at $q^k = 1$ and $q^k = \omega$ for all natural numbers k
- Singularites at $q^k = \omega$ for all natural numbers k actually occur
- $\bullet\,$ This implies essential singularities on approaching $z=1/\omega$ from below.
- There may also be a simple pole when the denominator is zero: this certainly happens when $\omega = 1$ and for some $\omega > 1$.
- These singularities should meet at the tricritical point.
- But how does one prove it!
- So they went to lunch ...

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The p	proof			

- Can find a functional equation for the functions $g_r^{(1)}$ which lead to a continued fraction expansion
- Use theory of continued fractions
- Worpitzky's theorem

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Variable flexibility

Final singularity diagram for IPDW



Interacting Partially Directed Walks

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But is it collapse?

Prellberg moves to Melbourne and then Owczarek moves to Melbourne

- Prellberg, Owczarek, Brak and Guttmann 1993 produced series using the recurrences for walks of length up to several thousand.
- They numerically verified the scaling predictions of Owczarek, Prellberg and Brak 1993

So what did Owczarek, Prellberg and Brak 1993 do?

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OPB 1993

- Made predictions for the scaling of properties above, below and around the collapse point.
- $\bullet\,$ Solved a semi-continuous variant of IPDW and showed explicitly the tricritical scaling around ω_t
- Generalised the solution of Brak, Guttmann, Whittington to distinguish horizontal to vertical steps
- Use perturbation expansions (non-rigorous) to demonstrate tricritical scaling in the discrete IPDW model
- Showed how the generating function of the semi-continuous model was a simple limit of the discrete model
- Connect the work of Zwanzig and Lauritzen and IPDW
- Relate SOS model of magnetic model interfaces and IPDW generating functions
- In an appendix solve a generalisation that distinguishes positive and negative vertical steps

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Scali	ng 1			

The following were found exactly for the semi-continuous model and verified for the discrete IPDW

- At high temperature $\omega<\omega_t$ we have $\gamma=$ 1, $\nu_{\parallel}=$ 1, $\nu_{\perp}=1/2$ and $\nu_r=0$
- At the collapse point precisely $\omega = \omega_t$ we have $\gamma \equiv \gamma_t^{direct} = 1/3$, $\nu_{\parallel} = 2/3$, $\nu_{\perp} = 1/3$ and $\nu_r = 1/3$
- $\bullet\,$ For low temperatures we have $\nu_{\parallel}=1/2,\,\nu_{\perp}=1/4$ and $\nu_r=1/2$

Later work by Owczarek (1993) shows the low temperature scaling of the partition function does not follow the usual form

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Singularity diagram: calculated from continued fractions



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Tricritical point scaling region



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Semicontinuous IPDW

- A variant is to allow the vertical sections of the walk be of any *Real* length rather than discrete
- Naturally horizontal and vertical "steps" are distinguished

Semi-continuous interacting partially directed walk



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Solution of the semi-continuous model

The solution can be written in terms of Bessel functions:

$$1 + G_{semi-cont}(x, y; \omega) = \sigma^{-1} \frac{J_{\lambda}(\sigma \lambda)}{J'_{\lambda}(\sigma \lambda)}$$

where $\sigma = \left(\frac{4x}{\beta J}\right)^{1/2}$ and $\lambda = \frac{\beta J}{\tau - \beta J}$ while $\omega = e^{\beta J}$ and $y = e^{-\tau}$ Near the tricritical point we have

$$G_{semi-cont}(x=1, y(\lambda); \omega(\zeta)) \approx -\left(\frac{\zeta}{1-\sigma^2}\right)^{1/2} \frac{\operatorname{Ai}(\lambda^{2/3}\zeta)}{\operatorname{Ai}'(\lambda^{2/3}\zeta)} \lambda^{1/3}$$

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Tricritical scaling

This gave us verification of the general scaling ansatz

$$G(z;\omega) \sim rac{1}{(z-z_t)^{\gamma_t}} \mathcal{S}\left(rac{\omega-\omega_t}{(z_t-z)^{\phi}}
ight)$$

where $z_t \equiv z_c(\omega_t)$ with $\gamma_t \equiv \gamma_t^{direct} = 1/3$ and the crossover exponent $\phi = 2/3$.

This is consistent with our calculated value of 1/2 for $\gamma_t^{\rm tangential}$ as we must have

$$\gamma_t^{\text{tangential}} = \gamma_t^{\text{direct}} / \phi$$

It also follows that the thermal exponent $\alpha = 2 - \frac{1}{\phi} = 1/2$.

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IPDW differentiating horizontal and vertical steps

Another variation solved was distinguishing horizontal and vertical steps with counting variables x and y: similar q series solution



Horizontal force interpretation not realised at the time however!

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The	final nail			

- In 1995 Prellberg rigorously proved uniform asymptotic results for *q*-Bessel functions in the context of the *Bar graph* polygon model.
- However the functions involved in IPDW are related
- So we left it at that after all, all the results were in the literature, though not in one place.

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Stretching polymer

- With the advent of instruments in the early naughties that can micromanipulate single polymer molecules there was a renewed interest in the behaviour of polymers when placed under a stress
- Rosa, Marenduzzo, Maritan, and Seno (2003) cleverly reinterpreted IPDW distinguishing horizontal and vertical steps as a model of stretching (horizontally) collapsing polymers.
- This can be done simply by substituting

x = hz, y = z with $h = e^{\beta f_x}$

• They plotted critical force-temperature curves and conjectured various exponents.

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IPDW differentiating horizontal and vertical steps



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Adding stiffness to collapsing polymers

- For ISAW it was seen by Bastolla and Grassberger (1997) that adding stiffness can change the collapse transition to first order
- Different in effect in different dimensions and needs sufficient stiffness
- Zhou, Zhou, Zhong-Can Ou-Yang, and Kumar (*Phys. Rev. Lett.* (2006) studied "Collapse Transition of Two-Dimensional Flexible and Semiflexible Polymers"
 - Actually considered IPDW modified
 - Used analytic approximation and Monte Carlo
 - Conjectured that the collapse transition becomes first order with any stiffness added

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Solut	tion		

Owczarek and Prellberg, J. Stat. Mech.: Theor. Exp., P11010:1-14, 2007 "Exact Solution of Semi-Flexible and Super-Flexible Interacting Partially Directed Walks"

The solution for the generating was found using the Temperley-like methodology:

$$1+G(z;h,\sigma,\omega)=\frac{(1-\omega)}{2}\left[\mathcal{H}(z,z\omega,hz^2(\omega-1))-\left(\frac{(1+\omega)}{2}+\frac{(1-\omega)}{2}\frac{hz}{1-hz(\sigma-1)}\right)\right]^{-1}$$

where

$$\mathcal{H}(y,q,t) = \frac{H(y,q,qt)}{H(y,q,t)} \quad \text{and} \quad \mathcal{H}(y,1,t) = \frac{1}{2y} \left[1 + y - t - \sqrt{(1+y-t)^2 - 4y} \right]$$

with

$$H(y,q,t) = \sum_{n=0}^{\infty} \frac{q^{\binom{n}{2}}(-t)^n}{(y;q)_n(q;q)_n}$$

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Solving along q = 1

Let $u = \omega/(\omega - h(\sigma - 1))$, then along the curve q = 1 the generating function has an algebraic singularity at

$$\omega_{a}(h) = \left(rac{\omega+h}{\omega-h}
ight)^{2}$$

and for u > 1 a simple pole at

$$\omega_{p}(h, u) = \frac{(\omega + uh)(\omega + 2h - uh)}{(\omega - uh)(\omega - 2h + uh)}$$

The singularities coincide for u = 1, ie. $\sigma = 1$.

So, minor change to the solution: this changes the singularity structure it seems ... lunch

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Interacting Partially Directed Walks

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Singularity diagram: no stiffness



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Singularity diagram: adding positive stiffness



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Singularity diagram: encouraging bends



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Exponents

Fully flexible case ($\Delta = 0$): we have a second-order collapse transition with

$$\gamma_t^{\text{tangential}} = \frac{1}{2} \qquad \gamma_t^{\text{direct}} = \frac{1}{3} \qquad \phi = \frac{2}{3}$$

Super-flexible case ($\Delta < 0):$ we have a second-order collapse transition with

$$\gamma_t^{\text{tangential}} = -\frac{1}{2} \qquad \gamma_t^{\text{direct}} = -\frac{1}{3} \qquad \phi = \frac{2}{3} \; ,$$

Semi-flexible case ($\Delta > 0$): first order transition.

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Scaling region 1

Using Lemma 4.3 from Prellberg (1995), a result completely analogous to Theorem 5.3 in Prellberg (1995) can be obtained for $\mathcal{H}(y, q, t)$, i.e. an asymptotic expansion in $q = 1 - \epsilon$ uniformly valid for all values of t and y, which reads

$$\mathcal{H}(y,1-\epsilon,t) = \frac{1}{2y} \left[1+y-t - \left(-\frac{\operatorname{Ai}'(\alpha \epsilon^{-2/3})}{\alpha^{1/2} \epsilon^{-1/3} \operatorname{Ai}(\alpha \epsilon^{-2/3})} \right) \sqrt{(1+y-t)^2 - 4y} \right] (1+O(\epsilon)) \ .$$

Here, $\alpha = \alpha(y, t)$ is a function of y and t which is known exactly. Near the tricritical point

$$\alpha(y,t) \sim \left(\frac{4}{1-(t-y)^2}\right)^{4/3} \frac{(1+y-t)^2-4y}{4}$$

for small $(1 + y - t)^2 - 4y$.

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Scaling region 2

$$\mathcal{H}(y, 1-\epsilon, t) \sim rac{1}{2y} \left[1+y-t+\epsilon^{1/3} rac{\mathsf{Ai}'(lpha\epsilon^{-2/3})}{\mathsf{Ai}(lpha\epsilon^{-2/3})} rac{(1-(t-y)^2)^{2/3}}{2^{1/3}}
ight]$$

The behaviour of this expression is determined by the function $f(z) = -\operatorname{Ai}'(z)/\operatorname{Ai}(z)$

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The function $f(z) = -\operatorname{Ai}'(z)/\operatorname{Ai}(z)$

- The large-z asymptotics allows for matching for $\epsilon \to 0$ and positive $\alpha.$
- For negative α, the argument of f is negative. As f(z) has a simple pole at z = -2.3381..., for any fixed α < 0 we have a pole at a finite value of ε.
- As α tends to zero, the locus of this pole scales as $\epsilon^{2/3}$.



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What next?



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The solution

The solution can be found in (you guessed it) Owczarek, Prellberg and Brak (1993) as

$$1 + G(x, y_+, y_-, \omega) = \frac{1 - \omega}{2} \left\{ \mathcal{H}(x, y_+, y_-, \omega) - (\frac{1 + \omega}{2} + \frac{1 - \omega}{2} x) \right\}^{-1}$$

where

$$\mathcal{H}(x, y_{+}, y_{-}, \omega) = \frac{(A_{0}^{+} + B_{0}^{+})(A_{1}^{+} - B_{1}^{+}) - (A_{0}^{-} + B_{0}^{-})(A_{1}^{-} - B_{1}^{-})}{(A_{0}^{+} + B_{0}^{+})(A_{0}^{+} - B_{0}^{+}) - (A_{0}^{-} + B_{0}^{-})(A_{0}^{-} - B_{0}^{-})}$$

and

$$\begin{aligned} A_r^{\pm} &= \sum_{m=0}^{\infty} \frac{x^{2m} (\omega - 1)^{2m} (q_+ q_-)^{m(m+r)} q_{\pm}{}^m}{\prod_{k=1}^m P[(q_+ q_-)^{k-1} q_{\pm}] P[(q_+ q_-)^k]} \\ B_r^{\pm} &= \sum_{m=0}^{\infty} \frac{x^{2m+1} (\omega - 1)^{2m+1} (q_+ q_-)^{m(m+r)} q_{\pm}{}^{r+m+1}}{P[(q_+ q_-)^m q_{\pm}] \prod_{k=1}^m P[(q_+ q_-)^{k-1} q_{\pm}] P[(q_+ q_-)^k]}. \end{aligned}$$

and $P[l] = (l-1)(l-\omega)$ Note that $q_+q_- = q^2$, and given that all the parameters are positive we have $q = \sqrt{q_+q_-}$. But what can we say about the singularity structure, phase transition, scaling etc ...

			Variable flexibility
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Conc	lusions		

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