The pressure of surface-attached polymers and vesicles

Thomas Prellberg[1] and Aleks Owczarek[2]

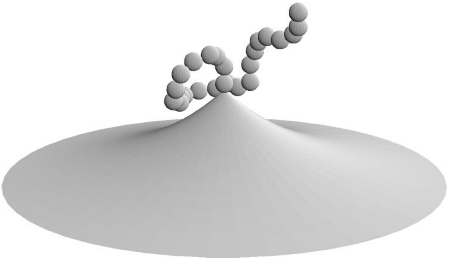
[1]Queen Mary University of London
[2]The University of Melbourne

Open Statistical Physics 2015

Topic Outline

Outline

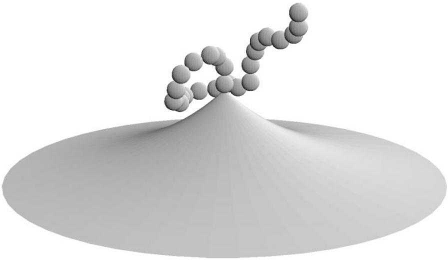
Surface-grafted polymers



A polymer grafted to a surface exerts pressure on it

Bickel *et al*, PRE **62** (2000) 1124

Surface-grafted polymers



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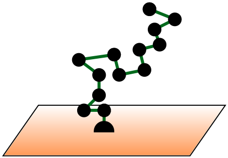
Related to change of entropy

From Polymer to Lattice Model

Coarse-grained “beads on a necklace”



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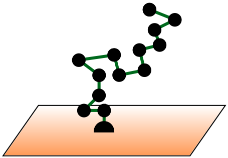
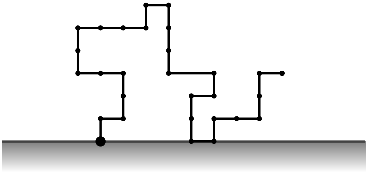
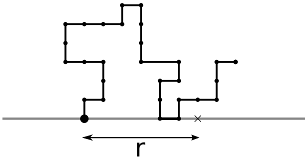


Self-avoiding walk on a regular lattice



Some Notation



C_n: number of n-step polymers

$C_n(r)$: number of n-step polymers avoiding site at distance r

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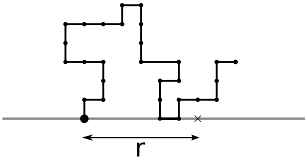

Pressure of polymer on surface

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$$P_n(r) = -\log \frac{C_n(r)}{C_n}$$

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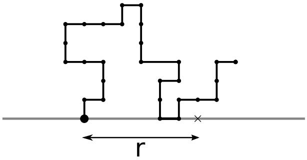

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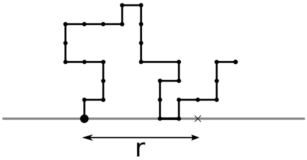

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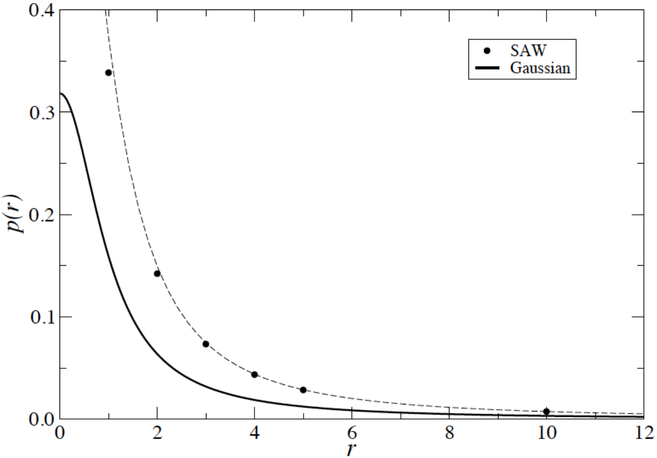
Gaussian chains (Bickel, 2000)

$$P_G(r) = \frac{\Gamma(d/2)}{\pi^{d/2}} \frac{1}{(r^2+1)^{d/2}}$$

SAW versus Gaussian chain



extrapolated from exact enumeration data up to $n = 59$, $r = 10$

Jensen *et al*, J Phys **46** (2013) 115004

Outline

Exactly Solvable Models

Directed walk models

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- Directed walks (both/one ends grafted)

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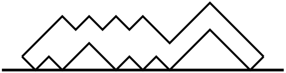
- Directed walks (both/one ends grafted)

- Pairs of directed walks



Exactly Solvable Models

Directed walk models

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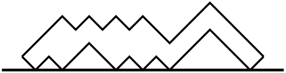
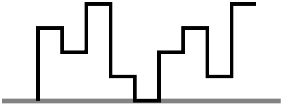
- Pairs of directed walks



- Partially directed walks



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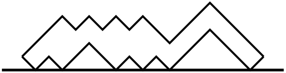

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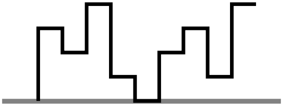

Moreover, add contact weights, area weights, nearest-neighbour interactions, . . .

Much activity ensued . . .

So far

- Directed walks with contacts

  E J Janse van Rensburg and TP, J. Phys. A **46** (2013) 115202

- Pairs of walks with contacts

  E J Janse van Rensburg and TP, J. Phys. A **46** (2013) 115202

- Directed walks with area

  A Owczarek and TP, J. Phys. A **47** (2014) 215001

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The next model to be done

- Interacting partially directed walks

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The next model to be done

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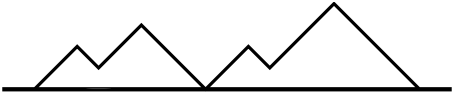
Also

- Rooted self-avoiding polygons

  F Gassoumov and E J Janse van Rensburg, J. Stat. Mech. (2013) P10005

Dyck paths

Directed walks with both ends tethered $\Leftrightarrow$ Dyck paths



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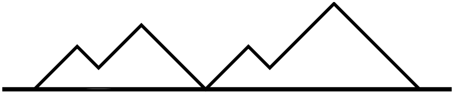

- $2n$-step Dyck paths are counted by the n-th Catalan number C_n

$$D_{2n} = C_n \equiv \frac{1}{n+1}\binom{2n}{n} \sim \frac{4^n}{\sqrt{\pi}n^{3/2}}$$

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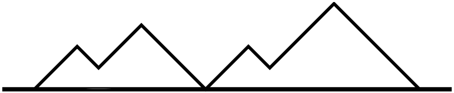

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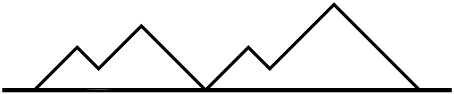
- Exclude paths touching the surface at distance $2r$

$$D_{2n}(r) = D_{2n} - D_{2r} D_{2n-2r}$$

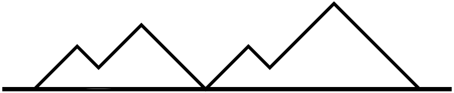
Dyck paths



- Compute pressure

$$P_{2n}(r) = \log \frac{D_{2n}(r)}{D_{2n}} = -\log \left(1 - \frac{C_r C_{n-r}}{C_n} \right)$$

Dyck paths



- Compute pressure

$$P_{2n}(r) = \log \frac{D_{2n}(r)}{D_{2n}} = -\log\left(1 - \frac{C_r C_{n-r}}{C_n}\right)$$

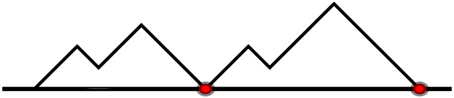
- Limiting pressure

$$P_{2n}(2r) \sim \frac{1}{\sqrt{\pi}(na(1-a))^{3/2}} \qquad r = na,\ n \to \infty$$

$$P(r) \sim \frac{1}{\sqrt{\pi} r^{3/2}} \qquad \text{first } n \to \infty, \text{ then } r \to \infty$$

Adsorbing Dyck paths

Surface contact weight z



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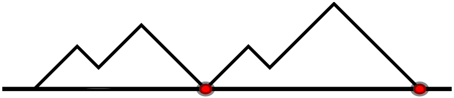

- Exact partition function

$$Z_n(z) = \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{4m+2}{n+2(m+1)} \binom{n}{\lfloor n/2 \rfloor + m} (z-1)^m$$

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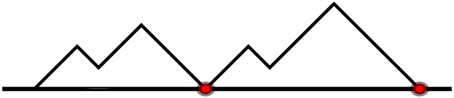

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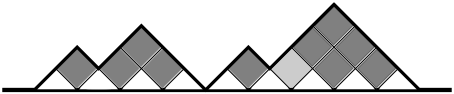
- Limiting pressure

$$P_n^D(z; 2\lfloor an/2 \rfloor) \simeq \begin{cases} \frac{8}{\sqrt{2\pi n^3 a^3 (1-a)^3}\ \log^2(z-1)}, & \text{if } z < 2; \\ \frac{\sqrt{2}}{\sqrt{\pi n a (1-a)}} & \text{if } z = 2; \\ \log(z-1) + \frac{A}{12na(1-a)(z-1)(z-2)}, & \text{if } z > 2; \end{cases}$$

for n even, with $A = (a^2 - a + 1)(z^4 + 8z^3 + 30z^2 - 32z + 16)$

Area-weighted Dyck paths

Dyck paths weighted by enclosed area, area weight q



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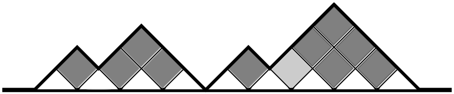

- Replace the n-th Catalan number C_n by $C_n(q)$

$$C_0(q) = 1\,, \quad C_{n+1}(q) = \sum_{k=0}^{n} q^k C_k(q) C_{n-k}(q) \quad n \geq 0$$

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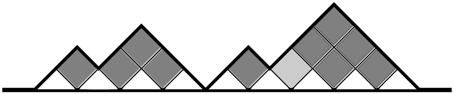

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- Pressure $P_{2n}(q,r)$ is now given by

$$P_{2n}(q,r) = -\log\left(\frac{C_n(q) - C_r(q) C_{n-r}(q)}{q C_n(q)}\right)$$

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$G(t, q)$ is fairly well understood, $C_n(q)$ much less

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- Continued fraction representation

$$G(t,q) = \cfrac{1}{1 - \cfrac{t}{1 - \cfrac{qt}{1 - \cfrac{q^2 t}{1 - \dots}}}}$$

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- Alternatively

$$G(t,q) = \frac{A_q(t)}{A_q(t/q)}$$

where

$$A_q(t) = \sum_{n=0}^{\infty} \frac{q^{n^2}(-t)^n}{\prod_{k=1}^{n}(1-q^k)}$$

is Ramanujan's Airy function

Scaling for $q \to 1$

Scaling function near $q = 1$ and $t = t_c(1) = 1/4$

$$f(s) = \lim_{q \to 1^-} \left(2 - (1-q)^{-1/3} G(1/4 - s(1-q)^{2/3}, q)\right) = -2\frac{\mathrm{Ai}'(4s)}{\mathrm{Ai}(4s)}$$

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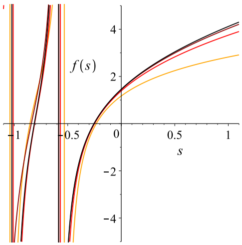

see talk by Nils Haug today, N Haug and TP, arXiv:1412.5108

Bulk pressure

Compute pressure in the bulk using surface contacts

- Weight surface contacts by z

$$G(t,q;z) = \cfrac{1}{1 - \cfrac{tz}{1 - \cfrac{qt}{1 - \cfrac{q^2 t}{1 - \dots}}}}$$

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- Equivalently

$$G(t,q;z) = \frac{1}{1 - tzG(qt,q)}$$

Bulk pressure

- Density of contacts $\rho(q)$ is related to singularity $t_c(q;z)$

$$\rho(q) = -\left.\frac{\partial \log t_c(q;z)}{\partial \log z}\right|_{z=1}$$

Bulk pressure

- Density of contacts $\rho(q)$ is related to singularity $t_c(q;z)$

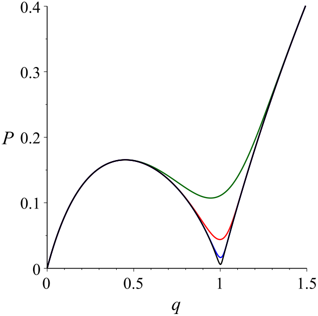
$$\rho(q) = -\left.\frac{\partial \log t_c(q;z)}{\partial \log z}\right|_{z=1}$$

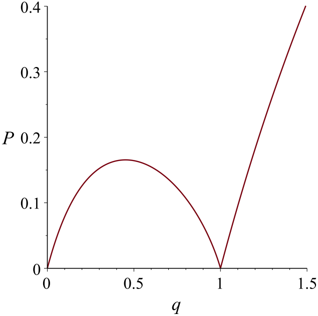
- We find for the pressure $P(q)$

$$P(q) = -\log(1-\rho(q)) + \log q$$

Bulk pressure

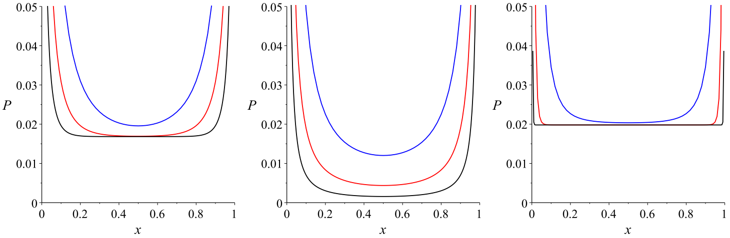
Bulk pressure for $n = 10$ to 80 (left) and in the TDL (right)





Pressure Profiles

Pressure profiles for $q = 0.98$ (left), 1.00 (center), and 1.02 (right)



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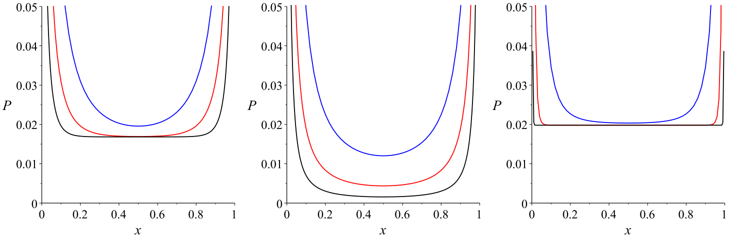

Rate of convergence: ρ^n (left), $n^{-1/2}$ (center), and ρ^{n^2} (right)

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Conclusion

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Simple lattice models still manage to give useful physical insight!