Exact solution of two friendly walks above a sticky wall with single and double interactions

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- Exact solutions of single and multiple directed walks models
- Recurrence and functional equation
- Rational, algebraic or non Differentially-finite (D-finite) solutions
- Multiple walks: Bethe Ansatz & Lindström-Gessel-Viennot
- LGV Lemma: multiple walks = determinant of single walk
- LGV problems result in generating functions that are D-finite

SOLVING FUNCTIONAL EQUATIONS

- Functional equation for an expanded generating function
- Uses an extra catalytic variable
- Answer is a ‘boundary’ value
- Fix catalytic variable $\rightarrow$ ‘bulk’ term disappears (Kernel method)
- Obstinate kernel method: multiple values of catalytic variable
- Solutions are not always D-finite

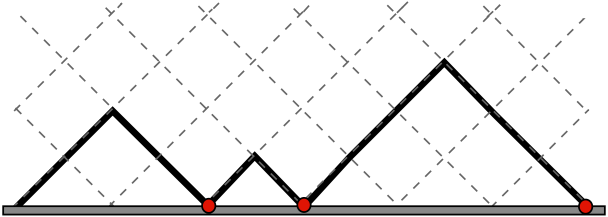
Polymer Adsorption

The physical motivation is the adsorption phase transition

- Second order phase transition with jump in specific heat
- Crossover exponent $\phi = 1/2$ for directed walks and SAW
- Order parameter is coverage of the surface by the polymer

Exact solution and analysis of single and multiple directed walk models exist

- Single Dyck path in a half space
- Energy $-\varepsilon_a$ for each time (number m_a) it visits the surface
- Boltzmann weight $a = \varepsilon_a / k_B T$



ADSORPTION: ONE DIRECTED WALK

A complete solution exists and the generating function is algebraic

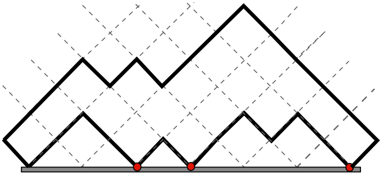
Consider the coverage

$$\mathcal{A} = \lim_{n\to\infty} \frac{\langle m_a \rangle}{n}$$

There exists a phase transition at a temperature T_a given by $a = 2$:

- For $T > T_a$ the walk moves away entropically and $\mathcal{A} = 0$
- For $T < T_a$ the walk is adsorbed onto the surface and $\mathcal{A} > 0$

Vesicle adsorption



- Exact solution of two directed walks joined making a simple "vesicle" (R. Brak *et al.* , *J. Stat. Phys.* **93**, 155 (1998))
- Vesicles with interactions for visits of the *bottom* walk to height 0 and height 1 (H. Lonsdale *et al.* , *J. Phys. A.: Math. and Theor.* **42** 1, (2009).)

Single second order transition — similar to the single walk adsorption transition

More motivation: SAW in a slit

- A motivation is a Monte Carlo study of ring polymers in a slit
- Here Both sides of the polygon interact with the surfaces of the slit
  J. Alvarez *et al.* *J. Phys. A.: Math. and Theor.* **41**, 185004 (2008)

(Our Model)

Directed vesicle where both walks can interact with a single surface

MODEL

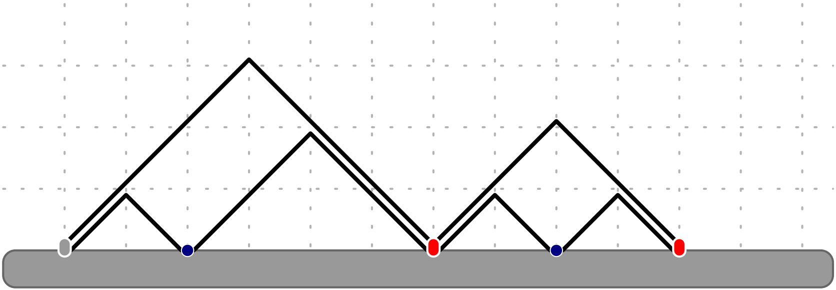


Figure: Two directed walks with single and "double" visits to the the surface.

- *energy* $-\varepsilon_a$ *for visits of the bottom walk only (single visits) to the wall,*
- *energy* $-\varepsilon_d$ *when both walks visit a site on the wall (double visits)*

- number of *single visits* to the wall will be denoted m_a,
- number of *double visits* will be denoted m_d.

The partition function:

$$Z_n(a,d) = \sum_{\widehat{\varphi} \ni |\widehat{\varphi}|=n} e^{(m_a(\widehat{\varphi})\cdot\varepsilon_a + m_d(\widehat{\varphi})\cdot\varepsilon_d)/k_B T}$$

where $a = e^{\varepsilon_a/k_B T}$ and $d = e^{\varepsilon_d/k_B T}$.

The thermodynamic reduced free energy:

$$\kappa(a,d) = \lim_{n\to\infty} n^{-1} \log\left(Z_n(a,d)\right).$$

To find the free energy we will instead solve for the generating function

$$G(a, d; z) = \sum_{n=0}^{\infty} Z_n(a, d) z^n.$$

The radius of convergence of the generating function $z_c(a, d)$ is directly related to the free energy via

$$\kappa(a, d) = \log(z_c(a, d)^{-1}).$$

Two order parameters:

$$\mathcal{A}(a, d) = \lim_{n\to\infty} \frac{\langle m_a \rangle}{n} \qquad \text{and} \qquad \mathcal{D}(a, d) = \lim_{n\to\infty} \frac{\langle m_d \rangle}{n},$$

FUNCTIONAL EQUATION

We consider walks φ in the larger set, where each walk can end at any possible height.

The expanded generating function

$$F(r,s;z) \equiv F(r,s) = \sum_{\varphi \in \Omega} z^{|\varphi|} r^{\lfloor \varphi \rfloor} s^{\lceil \varphi \rceil / 2} a^{m_a(\varphi)} d^{m_d(\varphi)},$$

where

- z is conjugate to the length $|\varphi|$ of the walk,
- r is conjugate to the distance $\lfloor \varphi \rfloor$ of the bottom walk from the wall and
- s is conjugate to *half* the distance $\lceil \varphi \rceil$ between the final vertices of the two walks.

G(a,d;z)= F(0,0)

FUNCTIONAL EQUATION

Consider adding steps onto the ends of the two walks

This gives the following functional equation

$$\begin{aligned} F(r,s) =& 1 + z\left(r + \frac{1}{r} + \frac{s}{r} + \frac{r}{s}\right)\cdot F(r,s) \\ & - z\left(\frac{1}{r} + \frac{s}{r}\right)\cdot [r^0]F(r,s) - z\frac{r}{s}\cdot [s^0]F(r,s) \\ & + z(a-1)(1+s)\cdot [r^1]F(r,s) + z(d-a)\cdot [r^1 s^0]F(r,s). \end{aligned}$$

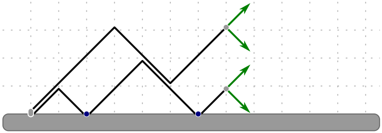


Figure: Adding steps to the walks when the walks are away from the wall.

The Kernel

Rewrite equation as "Bulk = Boundary"

$$K(r,s)\cdot F(r,s) = \frac{1}{d} + \left(1 - \frac{1}{a} - \frac{zs}{r} - \frac{z}{r}\right)\cdot F(0,s) - \frac{zr}{s}\cdot F(r,0) + \left(\frac{1}{a} - \frac{1}{d}\right)\cdot F(0,0)$$

where the *kernel* K is

$$K(r,s) = \left[1 - z\left(r + \frac{1}{r} + \frac{s}{r} + \frac{r}{s}\right)\right].$$

Recall, we want $F(0,0)$ so we try to find values that kill the kernel

The kernel is symmetric under the following two transformations:

$$(r,s) \mapsto \left(r, \frac{r^2}{s}\right), \qquad (r,s) \mapsto \left(\frac{s}{r}, s\right)$$

Transformations generate a family of 8 symmetries ('group of the walk')

$$(r,s), \left(r, \frac{r^2}{s}\right), \left(\frac{s}{r}, \frac{s}{r^2}\right), \left(\frac{r}{s}, \frac{1}{s}\right), \left(\frac{1}{r}, \frac{1}{s}\right), \left(\frac{1}{r}, \frac{s}{r^2}\right), \left(\frac{r}{s}, \frac{r^2}{s}\right), \text{ and } \left(\frac{s}{r}, s\right)$$

We make use of 4 of these which only involve positive powers of r.

This gives us four equations.

Following Bousquet-Mélou when $a = 1$ we form the simple alternating sum

$$Eqn1 - Eqn\ 2 + Eqn\ 3 - Eqn\ 4.$$

- When $a \neq 1$ one needs to generalise that approach
- Multiply by rational functions,

The form of the Left-hand side of the final equation being

$$a^2 rK(r,s)\left(sF(r,s) - \frac{r^2}{s}F\left(r, \frac{r^2}{s}\right) + \frac{Lr^2}{s^2}F\left(\frac{r}{s}, \frac{r^2}{s}\right) - \frac{L}{s^2}F\left(\frac{r}{s}, \frac{1}{s}\right)\right)$$

where

$$L = \frac{zas - ars + rs + zar^2}{zas - ar + r + zar^2}.$$

EXTRACTING THE SOLUTION $a = 1$

$$K(r,s) \cdot (\text{linear combination of } F) = \frac{r(s-1)(s^2+s+1-r^2)}{s^2}(1+(d-1)F(0,0)) - zd(1+s)sF(0,s) + \frac{zd(1+s)}{s^2}F\left(0,\frac{1}{s}\right).$$

- The kernel has two roots
- choose the one which gives a positive term power series expansion in z
- with Laurent polynomial coefficients in s:

$$\hat{r}(s;z) \equiv \hat{r} = \frac{s\left(1-\sqrt{1-4\frac{(1+s)^2z^2}{s}}\right)}{2(1+s)z} = \sum_{n\geq 0} C_n \frac{(1+s)^{2n+1}z^{2n+1}}{s^n},$$

where $C_n = \frac{1}{n+1}\binom{2n}{n}$ is a Catalan number.

EXTRACTING THE SOLUTION $a = 1$

- *Make the substitution* $r \mapsto \hat{r}$
- *rewrite to remove* z*:* $z = (\hat{r} + 1/\hat{r} + \hat{r}/s + s/\hat{r})^{-1}$.

Setting $r \mapsto \hat{r}$ gives

$$0 = ds^4 F(0,s) - dsF\left(0, \frac{1}{s}\right) - (s-1)(s^2+s+1-\hat{r}^2)(s+\hat{r}^2)\left(1+(d-1)F(0,0)\right)$$

Note coefficients of $F(0,s)$ and $F(0,1/s)$ are independent of $\hat{r}$.

Divide by equation by s *—* $F(0,0)$ *is a constant term in the variable* s*.*

SOLUTION FOR $a = 1$

Hence extracting the coefficient of s^1 gives

$$0 = -\left(1 + \sum_{n=0}^{\infty} \frac{12(2n+1)}{(n+2)^2(n+3)} C_n^2 z^{2n+2}\right) \cdot (1 + (d-1)F(0,0)) - d \cdot F(0,0).$$

Solving the above when $d = 1$ gives

$$G(1,1;z) = 1 + \sum_{n=0}^{\infty} \frac{12(2n+1)}{(n+2)^2(n+3)} C_n^2 z^{2n+2},$$

and hence for general d we have

$$F(0,0) = G(1,d;z) = \frac{G(1,1;z)}{d + (1-d)G(1,1;z)}.$$

$a = d$

Need to extract coefficients term by term in a to give

$$[a^k z^{2n}]F(0,0) = \sum_{k'=0}^{k} \frac{k'(k'+1)(2+4n-k'n-2k')}{(k'-1-n)(n+1)^2(-2n+k')(n+2)} \binom{2n-k'}{n}\binom{2n}{n}$$
$$= \frac{k(k+1)(k+2)}{(2n-k)(n+1)^2(n+2)} \binom{2n-k}{n}\binom{2n}{n}$$

which gives us

$$G(a,a) = \sum_{n\geq 0} z^{2n} \sum_{k=0}^{n} a^k \frac{k(k+1)(k+2)}{(n+1)^2(n+2)(2n-k)} \binom{2n}{n}\binom{2n-k}{n}.$$

Agrees with Brak *et al.* (1998) that used LGV

One can now consider $d \neq a$:

$$G(a,d;z) = \frac{aG(a,a;z)}{d+(a-d)G(a,a;z)}.$$

- Combinatorial structure the underlying the functional equation.
- Breaking up our configurations into pieces between double visits gives

$$G(a, d; z) = \frac{1}{1 - dP(a; z)}$$

where $P(a; z)$ is the generating function of so-called primitive factors.

- Rearranging this expression gives

$$P(a; z) = \frac{G(a, d; z) - 1}{dG(a, d; z)} = \frac{G(a, a; z) - 1}{aG(a, a; z)}.$$

- This allows us to calculate $P(a; z)$ from a known expression for $G(a, a; z)$

The phases determined by dominant singularity of the generating function

The singularities of $G(a,d;z)$ are

- *those of $P(a;z)$ and*
- *the simple pole at $1 - dP(a;z) = 0$ and*
- *the singularities of $P(a;z)$ are related to those of $G(a,a;z)$.*

There are two singularities of $G(a,a;z)$ giving rise to two phases:

- A desorbed phase: $\mathcal{A} = \mathcal{D} = 0$
- The bottom walk is adsorbed (an a-rich phase): $\mathcal{A} > 0$ with $\mathcal{D} = 0$

The simple pole in $1 - dP(a;z) = 0$ gives rise to the third phase

- Both walks are adsorbed and this is a d-rich phase: $\mathcal{D} > 0$, and $\mathcal{A} > 0$

Phase diagram

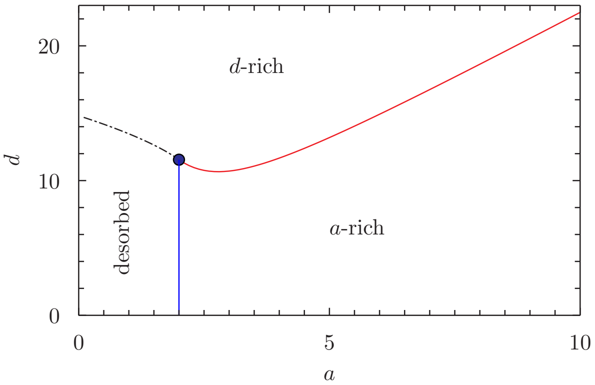


Figure: The first-order transition is marked with a dashed line, while the two second-order transitions are marked with solid lines. The three boundaries meet at the point $(a, d) = (a^*, d^*) = (2, 11.55\ldots)$.

Phase transitions

- The Desorbed to a-rich transition is
  - the standard second order adsorption transition
  - on the line $a = 2$ for $d < d^*$
- On the other hand the Desorbed to d-rich transition is first order
- While the a-rich to d-rich transition is also second order.

The other two phase boundaries are solutions to equations involving $G(a, a)$

The point where the three phase boundaries meet can be computed as

$$(a^*, d^*) = \left(2, \frac{16(8 - 3\pi)}{64 - 21\pi}\right)$$

Note that d^* is not algebraic.

Nature of the solution

Desorbed to d-rich transition occurs at a value of $d_c(a)$ for $a < 2$.
We found

$$d_c(1) = \frac{8(512 - 165\pi)}{4096 - 1305\pi}$$

which is not algebraic.

- *If generating function was D-finite the $d_c(1)$ must be algebraic*
- *Hence generating function is not D-finite*
- *it is a calculated in terms of one.*

FIXED ENERGY RATIO MODEL FAMILY

Family of models parameterised by $-\infty < r < \infty$ *where*

$$\varepsilon_d = r\varepsilon_a \qquad \text{and so} \qquad d = a^r$$

- $r = 2$ model has *two* phase transitions as temperature changed .
- At very low temperatures the model is in a d-rich phase
- while at high temperatures the model is in the desorbed state.
- At intermediate temperatures the system is in an a-rich phase.
- Both transitions are second-order with jumps in specific heat.

Conclusions

- Vesicle above a surface — both sides of the vesicle can interact
- Exact solution of generating function
- Obstinate kernel method with a minor generalisation
- Solution is not D-finite — LGV lemma does not apply directly
- There are two low temperature phases
- Line of first order transition and usual second order adsorption.
- Published in *J. Phys. A: Math. and Theor.* , 45 425002, (2012)