Area-weighed Dyck paths as vesicle models

an approach via q-deformed algebraic and linear functional equations

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Statistical Mechanics of Polymeric Systems

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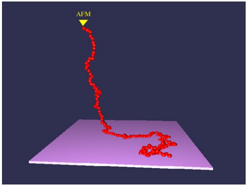
Topic Outline

Outline

Physical Motivation

Force-induced desorption (optical tweezers)

- Pulling a sticky polymer off a surface



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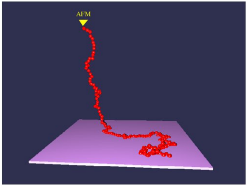
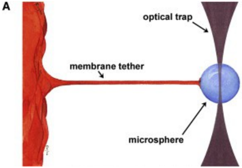
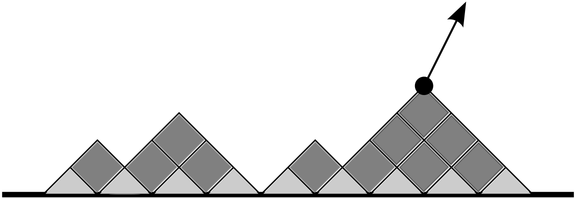


- Pulling on a membrane attached to a surface



Toy model: Dyck path



- $18 = 2n$ steps (n half length)
- $11 = m$ area (m rank function)
- $4 = h$ height (h length of final descent)

Outline

Mathematical Motivation

Compare two models of solving for the generating function

- Algebraic equation
- Linear functional equation in a "catalytic variable"

and their q-deformations

Mathematical Motivation

Compare two models of solving for the generating function

- Algebraic equation
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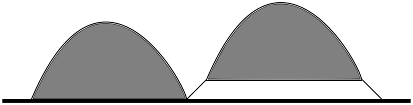
Generating function

$$G(t,q,\lambda) = \sum_{\pi \text{ Dyck path}} t^{n(\pi)} q^{m(\pi)} \lambda^{h(\pi)}$$

Outline

q-algebraic equation

Unique combinatorial decomposition of a Dyck path



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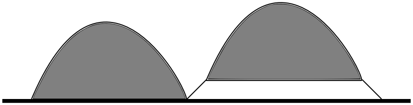


Functional equation

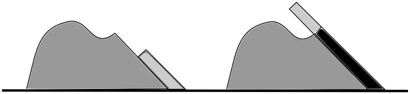
$$G(t,q,\lambda) = 1 + \underbrace{G(t,q,1)}_{\text{(a)}}\, t\, \underbrace{G(qt,q,\lambda)}_{\text{(b)}}\, \lambda$$

(a) left Dyck path does not contribute to final descent: $G(t,q,1)$

(b) raised right Dyck path increases area: $G(qt,q,\lambda)$

Outline

q-deformed linear functional equation



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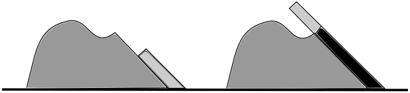
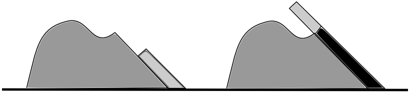


$$G(t,q,\lambda) = 1 + \underbrace{\frac{\lambda t}{1-q\lambda} G(t,q,{\color{red}1})}_{\text{(a)}} - \underbrace{\frac{q\lambda^2 t}{1-q\lambda} G(t,q,{\color{red}q}\lambda)}_{\text{(b)}}$$

q-deformed linear functional equation



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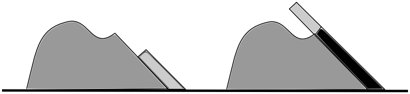
(a) add hooks irrespective of height

$$+G(t,q,1) \times (\lambda t + q\lambda^2 t + q^2\lambda^3 t + \dots)$$

q-deformed linear functional equation



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(a) add hooks irrespective of height

$$+G(t,q,1) \times (\lambda t + q\lambda^2 t + q^2\lambda^3 t + \dots)$$

(b) correct for overcounting

$$-G(t,q,q\lambda) \times (q\lambda^2 t + q^2\lambda^3 t + q^3\lambda^4 t + \dots)$$

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$$G(t,q,\lambda) = 1 + \lambda t G(t,q,1) G(qt,q,\lambda)$$

- $q = 1$ and $\lambda = 1$: quadratic equation

$$G(t,1,1) = \frac{1-\sqrt{1-4t}}{2t} = \frac{2}{1+\sqrt{1-4t}}$$

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- $q = 1$: back-substitution of $G(t,1,1)$ gives

$$G(t,1,\lambda) = \frac{2}{2-\lambda+\lambda\sqrt{1-4t}} = \sum_{l=0}^{\infty} \lambda^l t^l G(t,1,1)^l$$

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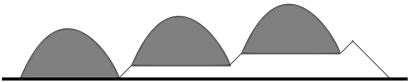

$l = 3$

q-deformed algebraic equation

- $q \neq 1$ and $\lambda = 1$: non-linear q-difference equation

$$G(t, q, 1) = 1 + \lambda t G(t, q, 1) G(qt, q, 1)$$

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- standard methods give

$$H(t, q) = \sum_{k=0}^{\infty} \frac{(-t)^k q^{k(k-1)}}{(q; q)_k}$$

where $(t; q)_k = \prod_{j=0}^{k-1}(1 - tq^j)$

q-deformed algebraic equation

General solution of

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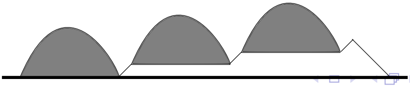
- combinatorial interpretation (with the power of hindsight)



First General Solution

We rewrite

$$G(t,q,\lambda)=\sum_{l=0}^{\infty}\prod_{k=0}^{l-1}\left(\lambda t q^k G(q^k t,1,1)\right)=\sum_{l=0}^{\infty}\lambda^l t^l q^{\binom{l}{2}}\frac{H(q^l t,q)}{H(t,q)}$$

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and find explicitly

$$G(t,q,\lambda)=\sum_{l=0}^{\infty}\lambda^l t^l q^{\binom{l}{2}}\frac{\sum_{k=0}^{\infty}\frac{(-q^l t)^k q^{k(k-1)}}{(q;q)_k}}{\sum_{k=0}^{\infty}\frac{(-t)^k q^{k(k-1)}}{(q;q)_k}}$$

Outline

linear functional equation

Functional equation

$$G(t,q,\lambda) = 1 + \frac{\lambda t}{1-q\lambda} G(t,q,1) - \frac{q\lambda^2 t}{1-q\lambda} G(t,q,q\lambda)$$

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"Kernel method": Rewrite

$$K(t,\lambda) G(t,1,\lambda) = 1 + \frac{\lambda t}{1-\lambda} G(t,1,1)$$

with Kernel

$$K(t,\lambda) = 1 + \frac{\lambda^2 t}{1-\lambda t}$$

Kernel method

Solving

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- LHS vanishes for some value $\lambda = \lambda_0$ such that $K(t,\lambda_0) = 0$

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- RHS gives

$$G(t,1,1) = \frac{\lambda_0 - 1}{1-\lambda_0 t} \quad \text{where} \quad \lambda_0 = \frac{1-\sqrt{1-4t}}{2t}$$

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- we find

$$G(t,1,\lambda) = \frac{1 + \frac{\lambda t}{1-\lambda} \frac{\lambda_0 t - 1}{\lambda_0 t}}{K(t,\lambda)}$$

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- we find

$$G(t,1,\lambda) = \frac{1 + \frac{\lambda t}{1-\lambda} \frac{\lambda_0 t - 1}{\lambda_0 t}}{K(t,\lambda)}$$

- eventually we recover the earlier solution

q-deformed linear functional equation

Now consider

$$G(t,q,\lambda) = 1 + \frac{\lambda t}{1-q\lambda} G(t,q,1) - \frac{q\lambda^2 t}{1-q\lambda} G(t,q,q\lambda)$$

for $q \neq 1$

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for $q \neq 1$

- mimic the Kernel method: rewrite

$$\left(1 + \frac{q\lambda^2 t}{1-q\lambda}\mathcal{Q}\right) G(t,q,\lambda) = 1 + \frac{\lambda t}{1-q\lambda} G(t,q,1)$$

  with an operator

$$(\mathcal{Q}G)(t,q,\lambda) = G(t,q,q\lambda)$$

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- we obtain formally

$$G(t,q,\lambda) = \left(1 + \frac{q\lambda^2 t}{1-q\lambda}\mathcal{Q}\right)^{-1} \left(1 + \frac{\lambda t}{1-q\lambda} G(t,q,1)\right)$$

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- now expand

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- we find

$$G(t,q,\lambda) \quad = \sum_{k=0}^{\infty} \left(-\tfrac{q\lambda^2 t}{1-q\lambda}\mathcal{Q}\right)^k \left(1 + \tfrac{\lambda t}{1-q\lambda} G(t,q,1)\right)$$

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- we find

$$\begin{aligned} G(t,q,\lambda) &= \sum_{k=0}^{\infty}\left(-\tfrac{q\lambda^2 t}{1-q\lambda}\mathcal{Q}\right)^k\left(1 + \tfrac{\lambda t}{1-q\lambda}G(t,q,1)\right) \\ &= \sum_{k=0}^{\infty}\frac{(-\lambda^2 t)^k q^{k^2}}{(q\lambda;q)_k}\left(1 + \tfrac{q^k\lambda t}{1-q^{k+1}\lambda}G(t,q,1)\right) \end{aligned}$$

q-deformed linear functional equation

- now expand

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- Letting $\lambda=1$ this simplifies to

$$G(t,q,1)=H(qt,q)-(H(t,q)-1)G(t,q,1)$$

and we recover

$$G(t,q,1)=H(qt,q)/H(t,q)$$

Second General Solution

We find explicitly

$$G(t,q,\lambda) = \sum_{k=0}^{\infty} \frac{(-q\lambda^2 t)^k q^{k(k-1)}}{(q\lambda;q)_k} - \frac{1}{\lambda} \sum_{k=1}^{\infty} \frac{(-\lambda^2 t)^k q^{k(k-1)}}{(q\lambda;q)_k} \frac{H(qt,q)}{H(t,q)}$$

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- no obvious combinatorial interpretation (yet)

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- no obvious combinatorial interpretation (yet)
- a clearly very different solution from

$$G(t,q,\lambda) = \sum_{l=0}^{\infty} \lambda^l t^l q^{\binom{l}{2}} \frac{H(q^l t,q)}{H(t,q)}$$

Why bother?

- Compare two fundamentally different ways of setting up and solving functional equations
- Algebraic decomposition does not always work
- The Kernel method approach is more general

Why bother?

- Compare two fundamentally different ways of setting up and solving functional equations
- Algebraic decomposition does not always work
- The Kernel method approach is more general
- However, there are cases when the Kernel method is fiendishly difficult to apply
- The q-deformation might actually make the functional equations easier to solve
- Work in progress . . .

Outline

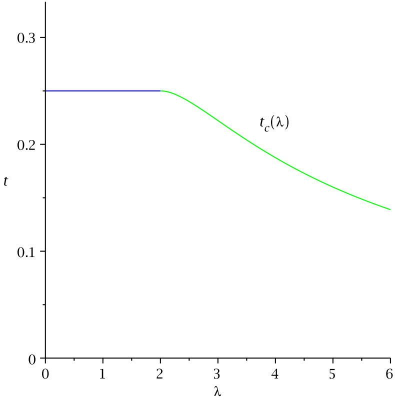
1. Physical Motivation

2. Mathematical Motivation
   - q-deformed algebraic equation
   - q-deformed linear functional equation

3. Solving the Functional Equations
   - q-deformed algebraic equation
   - q-deformed linear functional equation

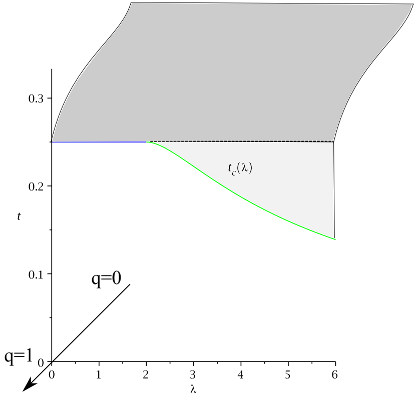
4. Back to Physics

The phase diagram for $q = 1$



- Phase transition at $\lambda = 2$

The phase diagram for general q



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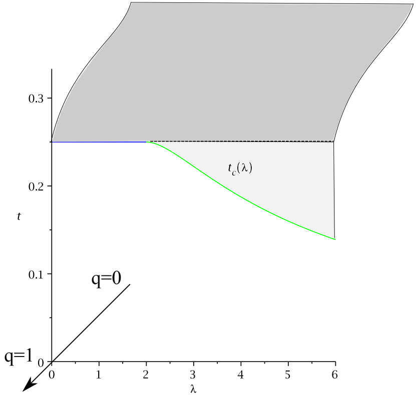

- $t_c(\lambda, q)$ independent of λ for $q < 1$
- Free energy jumps at $q = 1$ for $\lambda > 2$