Combinatorial Enumeration with the Kernel Method

1. Background (personal interest, no Kernel Method)

Want to understand classes of (self-avoiding) walks
- Mathematics: counting formulas, generating functions, ...
- Physics: lattice models of polymers, add weights

to study collapse, absorption, ...

Questions: thermodynamic limit, phase transitions, critical exponents, ...

Example 1 Self-avoiding walks on $\mathbb{Z}^2$ (SAW)

c_N = # of N-step walks starting at 0

hard combinatorial question

Proposition $\lim_{N\to\infty} c_N^{1/N} = \mu_{SAW}$ exists

Lemma (Subadditivity) If $a_{n+m} \leq a_n + a_m$

then $\lim_{n\to\infty} \frac{1}{n} a_n = \inf_{n\to\infty} \frac{1}{n} a_n$.

Remark: may be $-\infty$, need lower bound to prove finite limit

Proof (of proposition)

Concatenation: $c_{n+m} \leq c_n \cdot c_m$

take $a_n := \log c_n \rightsquigarrow a_{n+m} \leq a_n + a_m \rightsquigarrow \lim_{n\to\infty} \frac{1}{n} a_n = \inf_{n} \frac{1}{n} a_n$

$= \log \mu$

$c_n \geq 2^n$ (directed walks $\uparrow \rightarrow$)

$\rightsquigarrow \quad 2 \leq \mu_{SAW}$

$c_n \leq 3^n$ (random walks w/o reversal)

$\rightsquigarrow \quad \mu_{SAW} \leq 3$

Remarks: - refinement gives $c_N = \mu_{SAW}^{N + O(N^{1/2})}$

- known that $\frac{c_{N+2}}{c_N} \to \mu^2$, but $\frac{c_{N+1}}{c_N} \to \mu$ is open problem
- Physicists "know" that $c_N = \mu_{SAW}^N N^{\gamma - 1} A \, (1 + o(1))$

with $\gamma = 43/32$ (exact, non-rigorous)

$\mu_{SAW} = 2.68\ldots$ estimated up to 16 decimal places

- important connection to stochastic Loewner equation $SLE_{8/3}$

would lead to rigorous results if the scaling limit of SAW could be shown to be "conformally invariant".

Example 1a self-avoiding polygons on $\mathbb{Z}^2$ (SAP)

(counting translation-invariant equivalence classes)

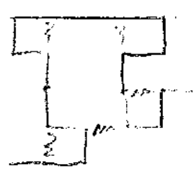
$$p_N = \mu_{SAP}^{N} N^{\alpha-2} B\,(1+o(1))$$

- $\mu_{SAP} = \mu_{SAW}$ (rigorous)
- $\alpha = \frac{1}{2}$ (non-rigorous)

Exercise prove existence of μ_{SAP}, give bounds

Example 2 interacting self-avoiding walks on $\mathbb{Z}^2$ (ISAW)

$c_{N,M}$ = # of N-step SAW with M interactions
(non-consecutive nearest-neighbours)



construct generating function (partition function)

$$Z_N(\omega) = \sum_M c_{N,M}\, \omega^M$$

$$\lim_{N\to\infty} \frac{1}{N} Z_N(\omega) = K(\omega)$$

(

<u>translation to physics:</u> $\omega = e^{-\beta J}$ Boltzmann weight

where $\beta = \frac{1}{k_B T}$ with T temperature, k_B Boltzmann constant.

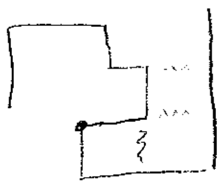
weight of a walk with m interactions has energy $E = mJ$:

$$\omega^m = e^{-\beta m J} = e^{-\beta E}$$

attractive interactions: $J < 0$, $E < 0$, $\omega > 1$.

free energy $f(T)$: $K(\omega) = -\frac{1}{k_B T} f(T)$, $\log \omega = -\frac{1}{k_B T} J$

existence of $K(\omega)$ is proved for $\omega \leq 1$:



$$Z_{N+M}(\omega) \leq Z_N(\omega)\, Z_M(\omega)$$

proof breaks down for $\omega > 1$ (self-avoidance & interactions have opposite effect)

$\rightsquigarrow$ $K(\omega)$ not rigorously known to exist.

<u>Exercise:</u> prove existence of $K(\omega)$ for interacting SAP for $\omega > 0$

Physicists "know" much more: $\exists\, \omega_c$ such that

$$Z_N(\omega) \sim A(\omega)\, \mu(\omega)^N N^{\gamma - 1} \quad \text{for } \omega < \omega_c$$

$$Z_N(\omega_c) \sim A(\omega_c)\, \mu(\omega_c)^N N^{\gamma_t - 1} \quad \text{for } \omega = \omega_c$$

$$Z_N(\omega) \sim A(\omega)\, \mu(\omega)^N \mu_s(\omega)^{N^{1/2}} N^{\gamma_- - 1} \quad \text{for } \omega > \omega_c$$

$\mu(\omega)$ is continuous for $\omega \geq 0$

$\mu(\omega)$ is real-analytic for $\omega < \omega_c$ and $\omega > \omega_c$

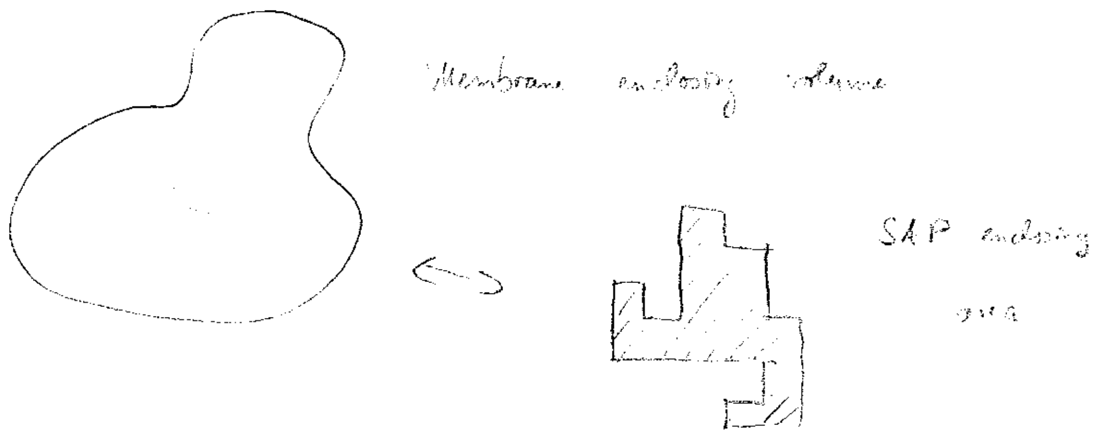
"<u>PHASE TRANSITION</u>" at $\omega = \omega_c$ (in literature: Θ-point)

moreover: intricate cross-over behaviour for ω near ω_c.

Huge gap between physicists' knowledge and mathematicians' rigour.

→ Need for alternative walk models that can be analyzed rigorously.

<u>Example 3</u> Lattice models of vesicles (vesiculum = bubble)



$c_{N,M}$ # of SAPs with perimeter N enclosing area M

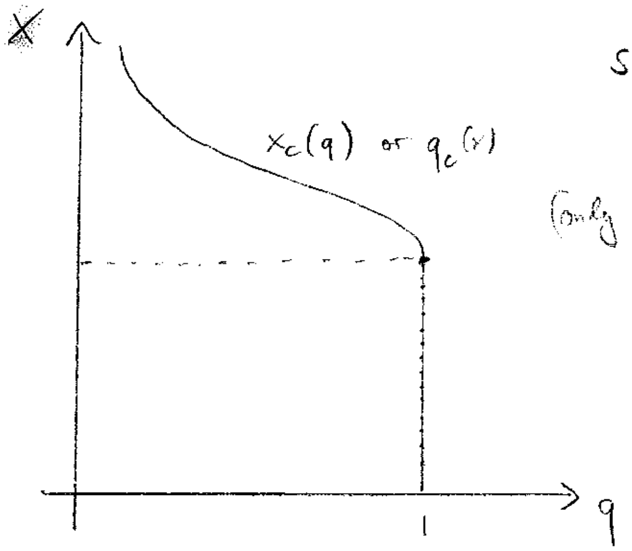
$$Z_N(q) = \sum_M{}' c_{N,M}\, q^M \qquad \text{finite-perimeter part. function}$$

$$Q_M(x) = \sum_N{}' c_{N,M}\, x^N \qquad \text{finite area part. function}$$

or

$$G(x,q) = \sum_{N,M}{}' c_{N,M}\, x^N q^M \qquad \text{"grand-canonical" partition function}$$

$$= \sum_N{}' Z_N(q)\, x^N = \sum_M{}' Q_M(x)\, q^M$$



Singularity diagram

(only closest singularity to the origin)

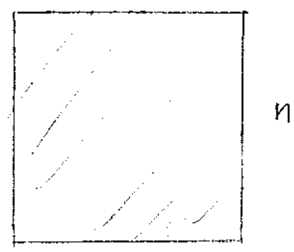
$$\lim_{N\to\infty} Z_N^{1/N}(q) = \frac{1}{x_c(q)} \qquad \lim_{n\to\infty} Q_n^{1/n}(x) = \frac{1}{q_c(x)}$$

(N even)

<u>Exercise</u>: prove existence of $x_c(q)$ for SAP with $q>0$

$$x_c(1) = \frac{1}{\mu_{SAW}}$$

$x_c(q) = 0$ for $q > 1$:



$$Z_{4n}(q) \geq q^{n^2}$$

jump of $x_c(q)$ at $q=1$: phase transition

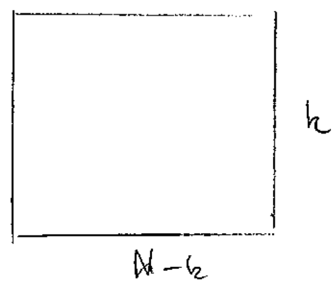
<u>Theorem</u>

$$Z_{2N}(q) = \frac{1}{\prod_{k=1}^{\infty}(1-q^{-k})^4} \sum_{k=-\infty}^{\infty} q^{k(N-k)} \left(1+O(\rho^{+N})\right)$$

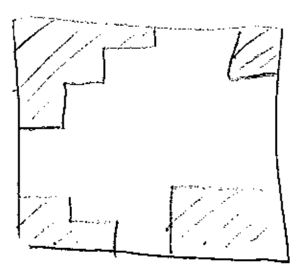
for some $0<\rho<1$

<u>Idea of proof</u>: for $q>1$, dominating polygons are close to rectangles:

$$R_N(q) = \sum_{k=1}^{N-1} q^{k(N-k)}$$



corrections to $R_N(q)$ come from "missing corners".



GF for corner is area-GF for Ferrer's diagram $\dfrac{1}{\prod_{k=1}^{\infty}(1-q^{k})} = \dfrac{1}{(q;q)_\infty}$

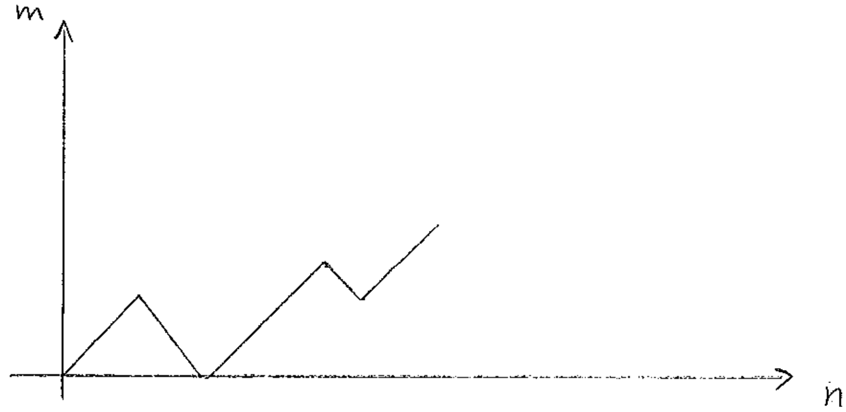
removing four corners (ignoring overlaps) does not change the perimeter: multiply by $\dfrac{1}{(q^{-1};q^{-1})_\infty^4}$

$$Z_{2N}(q) \approx \frac{1}{(q^{-1};q^{-1})_\infty^4} \sum_{k=\cancel{1}\,-\infty}^{\cancel{N-1}\,\infty} q^{k(N-k)} .$$

← exp. small error

The rest is hard estimates.

2. Yet another enumeration of Dyck paths (walks on $\mathbb{N}_0$)



$C_{N,M}$ # of N-step walks ending at position M

- recurrence (semi-infinite transfer matrix) $\begin{pmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & 1 & 0 & 1 & \\ & & 1 & 0 & 1 \\ & & & 1 & 0 \\ & & & & \ddots \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}$

  + related tricks

- reflection principle

- here: functional equation

$$G(x,t) = \sum_{N,M} C_{N,M}\, t^N x^M$$

$$C_{0,M} = \delta_{M,0} \qquad C_{N+1,M} = \begin{cases} C_{N,M-1} + C_{N,M+1} & M > 0 \\ C_{N,M+1} & M = 0 \end{cases}$$

leads to

$$G(x,t) = 1 + t\left(x\, G(x,t) + \frac{1}{x}\, G(x,t) \right)$$

$$- t\, \frac{1}{x}\, G(0,t)$$

here: correction of overcounting