Formation of facets in an equilibrium model of surface growth

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Technion

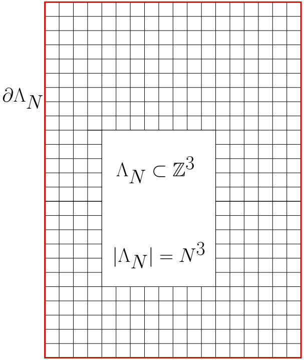
December 2011

[1] Based on joint works with Senya Shlosman

Plan of the talk

- Low temperature 3D Ising model, Wulff shapes and (unknown) structure of microscopic facets.
- Facets on SOS surfaces.
- Effective model of microscopic facets.
- Results and proofs.

3D Ising model



The Gibbs State

$$-\mathcal{H}_N^- = \frac{1}{2}\sum_{x\sim y}\sigma_x\sigma_y - \sum_{x\in\partial\Lambda_N}\sigma_x$$

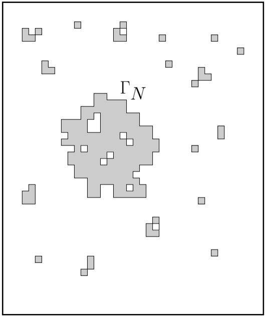
$$\mathbb{P}_{N,\beta}^-(\sigma) \sim \mathrm{e}^{-\beta\mathcal{H}_N^-}$$

Low Temperature $\beta \gg 1 \ \Rightarrow m^*(\beta) > 0$.
Phase Segregation: Fix $m > -m^*$ and consider

$$\mathbb{P}_{N,\beta}^{m,-}(\cdot) = \mathbb{P}_{N,\beta}^-\left(\cdot \mid \sum \sigma_x = mN^3\right).$$

Microscopic Wulff shape

Typical Picture under $\mathbb{P}^{m,-}_{N,\beta}$

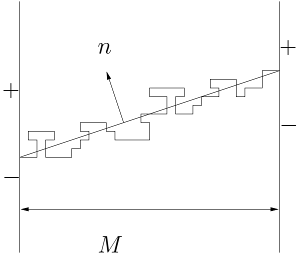


Volume of the microscopic Wulff droplet

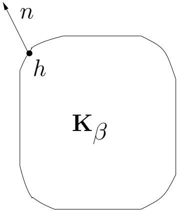
$$|\Gamma_N| \approx \frac{m+m^*}{2}N^3$$

Theorem (Bodineau, Cerf-Pisztora): As $N \to \infty$ the scaled shape $\frac{1}{N}\Gamma_N$ converges to the *macroscopic* Wulff shape.

Surface Tension and Macroscopic Wulff Shape



$$\tau_\beta(n) = -\lim_{M\to\infty} \frac{|\sin n|}{M^2} \log \frac{Z_M^\pm}{Z_M^-}.$$

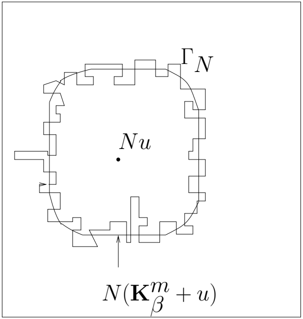


$$\tau_\beta = \max_{h\in\partial\mathbf{K}_\beta} h\cdot n$$

Dilated Wulff Shape

$$\mathbf{K}_\beta^m = \left(\frac{m+m^*}{2|\mathbf{K}_\beta|}\right)^{1/3} \mathbf{K}_\beta$$

Bodineau, Cerf-Pisztora Result



Define (on unit box $\Lambda \subset \mathbb{R}^3$)

$$\phi_N(t) = \mathbb{1}_{\{Nt \in \Gamma_N\}} - \mathbb{1}_{\{Nt \notin \Gamma_N\}}.$$

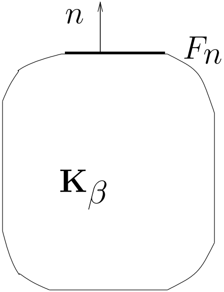
Define

$$\chi^m(t) = \mathbb{1}_{\left\{t \in \mathbf{K}_\beta^m\right\}} - \mathbb{1}_{\left\{t \notin \mathbf{K}_\beta^m\right\}}$$

Then, under $\left\{\mathbb{P}_{N,\beta}^{m,-}\right\}$,

$$\lim_{N\to\infty} \min_u \|\phi_N(\cdot) - \chi^m(u + \cdot)\|_{\mathbb{L}_1(\Lambda)} = 0$$

Macroscopic Facets



τ_β - support function of $\mathbf{K}_\beta$. Then

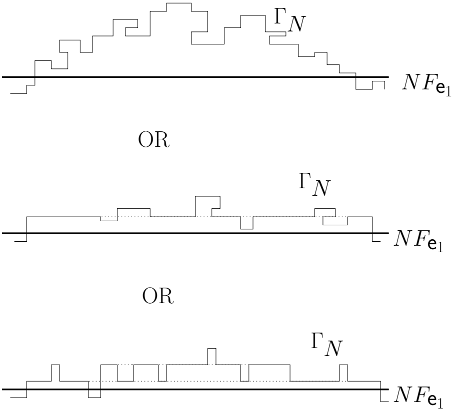
$$F_n = \partial\tau_\beta(n).$$

Set e_i - lattice direction. Dobrushin '72, Miracle-Sole '94:

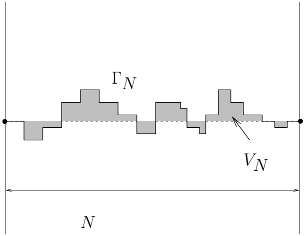
For $\beta \gg 1$ F_{e_i} is a proper 2D facet

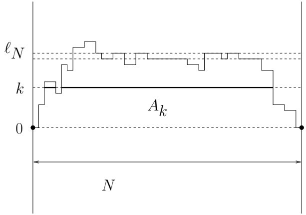
Microscopic Facets

Zooming Bodineau, Cerf-Pisztora picture, what happens?



SOS Model





Bodineau, Schonmann, Shlosman '05

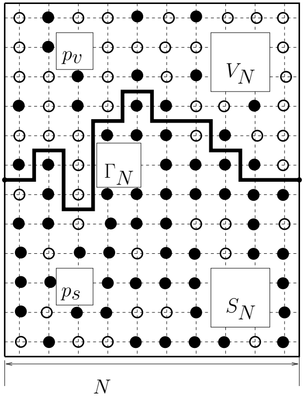
$$\mathbb{P}_N\left(\Gamma_N = \gamma\right) \sim \mathrm{e}^{-\beta|\gamma|}$$
$$\mathbb{P}_N^m\left(\cdot\right) = \mathbb{P}_N\left(\cdot \,\middle|\, V_N \geq mN^3\right)$$

Result: There exists $a(\beta) \searrow 0$ such that

$$\ell_N = \max\left\{k : A_k \geq a(\beta)N^2\right\}$$

satisfies $A_{\ell_N - 1} \geq (1 - a(\beta))N^2$.

Effective Model of Microscopic Facets



Configuration:

$$\left(\Gamma_N, \{\xi_i^v\}_{i\in V_N}, \{\xi_j^s\}_{j\in S_N}\right).$$

Total number of particles:

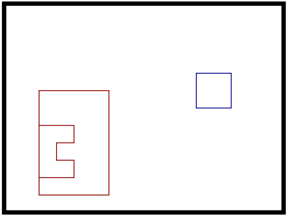
$$\Xi_N = \sum_{i\in V_N} \xi_i^v + \sum_{j\in S_N} \xi_j^s$$

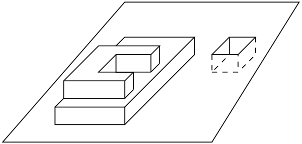
- $|\Gamma|$ - area of Γ
- $\mathbb{B}_p(\xi) = p^\xi(1-p)^{1-\xi}$
- β large

Probability Distribution:

$$\mathbb{P}_N(\Gamma, \xi^v, \xi^s) \propto \mathrm{e}^{-\beta|\Gamma|} \prod_{i\in V_N} \mathbb{B}_{p_v}(\xi_i^v) \prod_{j\in S_N} \mathbb{B}_{p_s}(\xi_j^s).$$

Contour Representation of Γ



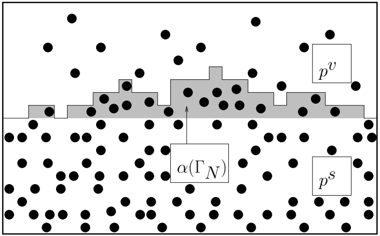


- Orientation of contours: Positive and negative (holes)
- $\alpha(\gamma)$ - signed area.
- $|\gamma|$ - length.
- Compatibility $\gamma \sim \gamma'$

For $\Gamma = \{\gamma_i\}$

$$|\Gamma| \sim \sum |\gamma_i|, \; \alpha(\Gamma) \triangleq \sum \alpha(\gamma_i)$$

Creation of Facets



$\delta = 2(p^s - p^v) > 0$

Ξ_N - total number of particles

$$\mathbb{E}_N(\Xi_N) = \frac{p^s + p^v}{2} N^3 \triangleq pN^3$$

Consider

$$\mathbb{P}_N^a(\cdot) = \mathbb{P}_N\left(\cdot \middle| \Xi_N = pN^3 + aN^2\right)$$

Surface Tension: $\log \mathbb{P}\left(\alpha(\Gamma_N) = bN^2\right) \approx -N$.

Bulk Fluctuations: $\mathbb{E}_N\left(\Xi_N \middle| \alpha(\Gamma_N)\right) = pN^3 + \delta N^2 \alpha(\Gamma_N)$.

$$\log \mathbb{P}_N\left(\Xi_N = pN^3 + aN^2 \middle| \alpha(\Gamma_N) = bN^2\right) \cong -\frac{(aN^2 - \delta bN^2)^2}{N^3 D}.$$

where $D = p^s(1 - p^s) + p^v(1 - p^v)$.

Reduction to Large Contours

Fix $\beta \gg 1$. Bulk fluctuations simplify analysis of $\mathbb{P}_N^a$. Recall the contour representation $\Gamma = \{\gamma_i\}$.

Lemma 1 (No intermediate contours). $\forall a > 0$ there exists $\epsilon = \epsilon(a) > 0$ such that

$$\mathbb{P}_N^a \left(\exists \gamma_i : \frac{1}{\epsilon} \log N \leq |\gamma_i| \leq \epsilon N \right) = o(1).$$

Lemma 2 (Irrelevance of small contours)

$$\mathbb{P}_N^a \left(\left| \sum \alpha(\gamma_i) \mathbb{1}_{\{|\gamma_i| \leq \epsilon^{-1} \log N\}} \gg N \right) = o(1).$$

Definition: γ is large if $|\gamma| \geq \epsilon N$.

Cluster Expansion and Reduced Model

A. Fix $a > 0$ and forget about intermediate contours $\frac{1}{\epsilon}\log N \leq |\gamma| \leq \epsilon N$.
B. Expand with respect to small contours $|\gamma| \leq \frac{1}{\epsilon}\log N$.

For $\Gamma = \{\gamma_i\}$ collection of large contours the effective weight is

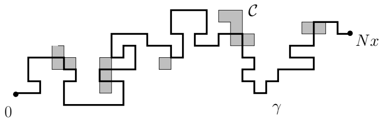
$$\hat{\mathbb{P}}_N(\Gamma) \propto \exp\left\{-\beta \sum |\gamma_i| - \sum_{\mathcal{C} \not\sim \Gamma} \Phi_\beta(\mathcal{C})\right\}.$$

The family of clusters $\mathcal{C}$ depends on N and a. However the cluster weights $\Phi_\beta(\mathcal{C})$ remain the same. The corrections are negligible: For all β sufficiently large $\exists\, \nu(\beta) \nearrow \infty$ such that $\sup_{\mathcal{C} \neq \emptyset} \mathrm{e}^{\nu|\mathcal{C}|}|\Phi_\beta(\mathcal{C})| \leq 1$.

Reduced Model of Large Contours and Bulk Particles:

$$\hat{\mathbb{P}}_N(\Gamma, \xi^v, \xi^s) = \hat{\mathbb{P}}_N(\Gamma) \prod_{i \in \hat{V}_N} \mathbb{B}_{p_v}(\xi_i^v) \prod_{j \in \hat{S}_N} \mathbb{B}_{p_s}(\xi_j^s)$$

Surface Tension and Variational Problem



$$w_\beta(\gamma) = \mathrm{e}^{-\beta|\gamma| - \sum_{\mathcal{C} \not\sim \gamma} \Phi_\beta(\gamma)}$$

$$G_\beta(Nx) = \sum_{\gamma:0\to Nx} w_\beta(\gamma).$$

$$\tau_\beta(x) = -\lim_{N\to\infty} \frac{1}{N} \log G_\beta(Nx).$$

$$\tau_\beta(\gamma) = \int_\gamma \tau_\beta(n_s)\mathrm{d}s.$$

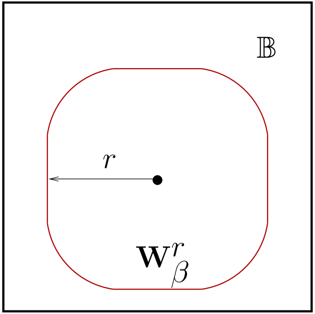
Macroscopic Variational Problem

$\mathbb{B} = [0,1]^2$ unit box. $\gamma_1, \dots, \gamma_n$ is a nested family of loops inside $\mathbb{B}$: If for $i \neq j$ either $\gamma_i \subseteq \gamma_j$ or $\gamma_j \subseteq \gamma_i$ or $\gamma_i \cap \gamma_j = \emptyset$. Recall $\delta = 2(p^s - p^v)$ and $D = p^v(1-p^v) + p^s(1-p^s)$.

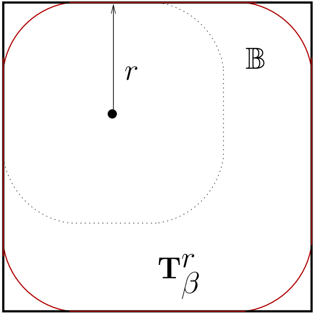
$$(\mathrm{VP})_a \qquad \min_b \left\{ \frac{(a-\delta b)^2}{D} + \min_{\alpha(\gamma_1)+\cdots+\alpha(\gamma_n)=b} \sum \tau_\beta(\gamma_i) \right\}.$$

Solutions to $(\mathrm{VP})_a$

All solutions $\bar{\gamma}^* = (\gamma_1^*, \dots, \gamma_n^*)$ form regular stacks: $\gamma_1^* \supseteq \gamma_2^* \supseteq \cdots \supseteq \gamma_n^*$.
Optimal loops γ_i^* are of two types:



Wulff shape of radius r

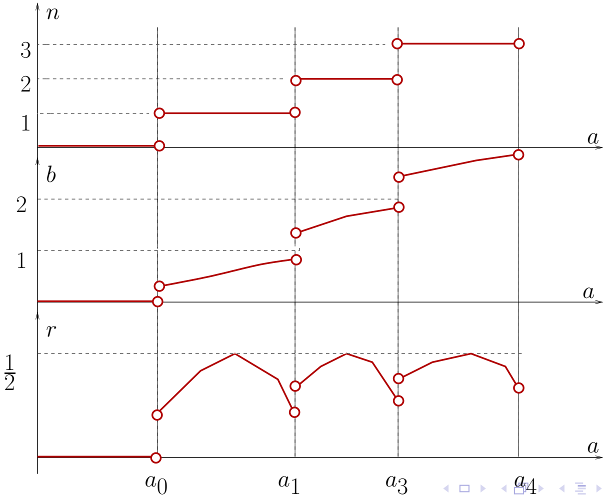


Wulff TV of radius r

Radius $r \le \frac{1}{2}$ is fixed for $\bar{\gamma}^*$: Either (a) $\gamma_1^* = \cdots = \gamma_n^* = \mathbf{T}_\beta^r$ or (b) $\gamma_1^* = \cdots = \gamma_{n-1}^* = \mathbf{T}_\beta^r$ and $\gamma_n^* = \mathbf{W}_\beta^r$.

1st Order Transition in the Variational Problem

Let $\bar{\gamma}^* = (\gamma_1^*, \ldots, \gamma_n^*)$ be a solution to $(\mathrm{VP})_a$.
Define $n = n(a)$, $b = b(a) = \sum_i \alpha(\gamma_i^*)$ and $r = r(a)$. Then:

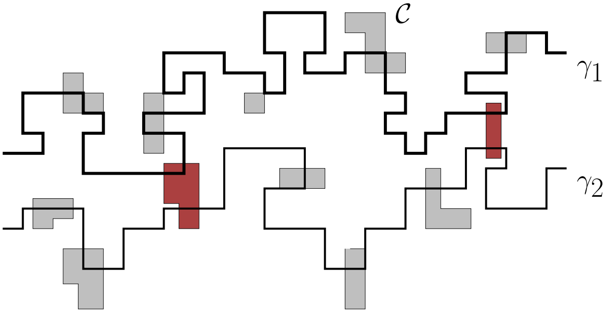


1st Order Transition in the Microscopic Model

Theorem. Fix β large. Then there exist $0 < a_1 < a_2 < a_3 < \dots$ such that $\forall a \in (a_n, a_{n+1})$ typical configurations under $\mathbb{P}_N^{a_N}$; where $a_N = \lfloor N^3 a \rfloor$, contain exactly n large contours, which are close in shape to $N\gamma_1^*, \dots, N\gamma_n^*$.

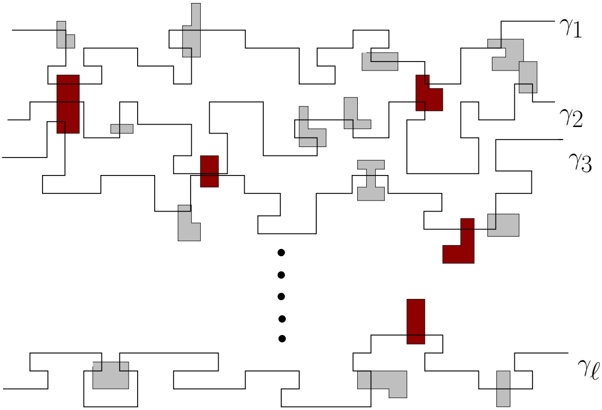
Remark: 1st order transition - spontaneous appearance of a droplet of linear size $N^{2/3}$ in the context of the 2D Ising model was originally established by Biskup, Chayes and Kotecky CMP'03. Because of large bulk fluctuations in our model, their result is more difficult for $n = 1$, but for $n = 2, 3, 4, \dots$ large contours in our model start to interact, and a refined control is needed for deriving appropriate upper bounds. There are two levels of difficulty:
(a) Controlling interactions between two large contours.
(b) For β fixed, controlling interactions for arbitrary fixed number of large contours as $N \to \infty$.

Interaction Between 2 Contours



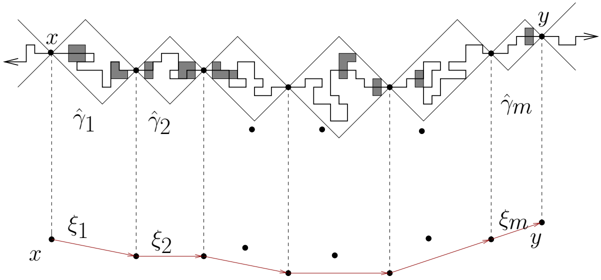
$$\sum_{\mathcal{C} \not\sim \gamma_1 \cup \gamma_2} \Phi_\beta(\mathcal{C}) = \sum_{\mathcal{C} \not\sim \gamma_1} \Phi_\beta(\mathcal{C}) + \sum_{\mathcal{C} \not\sim \gamma_2} \Phi_\beta(\mathcal{C}) - \sum_{\mathcal{C} \not\sim \gamma_1 \cap \gamma_2} \Phi_\beta(\mathcal{C})$$

Interaction Between ℓ Contours



Effective Random Walk Representation of G_β

Portion of a Contour Between x and y



$$\mathrm{e}^{\tau_\beta(y-x)} G_\beta(y-x) \cong \sum_m \sum_{\hat{\gamma}_1,\dots\hat{\gamma}_m} \prod \rho_\beta(\hat{\gamma}_i)$$

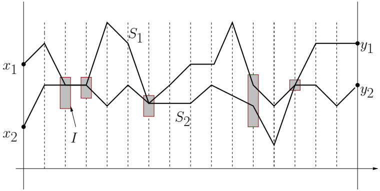
- $\{\rho_\beta(\cdot)\}$ is a probability distribution on the set of irreducible animals.
- $\xi_1 = (T_1, X_1), \xi_2 = (T_2, X_2), \dots$ steps of the effective random walk.

Attraction vrs Repulsion: Two Walks

• $S(n) = S(0) + \sum_1^n X_\ell$, where $X_\ell \in \mathbb{Z}$ are i.i.d. with exponential tails.
• $S_1(\cdot), S_2(\cdot)$ are two independent copies starting at $\underline{x} = (x_1, x_2)$ and ending (time n) at $\underline{y} = (y_1, y_2)$.
• Repulsion: Via event $\mathcal{R}_n^+ = \{S_1(\ell) \geq S_2(\ell)\ \forall \ell = 0, 1, 2, \dots, n\}$
• Attraction: Via potential

$$\Phi_{\beta,n}(\underline{S}) = \sum_{\ell=1}^{n} \sum_{I \supset \underline{S}(\ell)} \phi_\beta(|I|),$$

and $\phi_\beta(m) \leq \mathrm{e}^{-c(\beta)m}$ with $c(\beta) \nearrow \infty$.



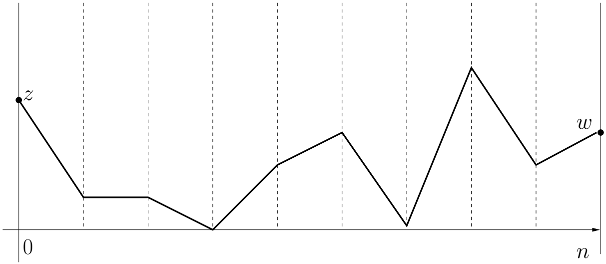
Lemma. For all β large enough

$$\mathbb{E}_{\underline{x}}\left(\mathrm{e}^{\Phi_{\beta,n}(\underline{S})}; \mathcal{R}_n^+; \underline{S}(n) = \underline{y}\right) \leq 1$$

uniformly in $\underline{x}, \underline{y}$ and $n \geq n_0$.

Attraction vrs Repulsion: Two Walks

Proof: $Z(\ell) = S_1(\ell) - S_2(\ell)$. Input (e.g. Allili and Doney '99; Campanino, Ioffe and Louidor '10)



$$\mathbb{P}_z\left(\mathcal{R}_n^+; Z(n) = w\right) \lesssim \frac{(1+z)(1+w)}{n}\,\mathbb{P}_z\left(Z(n) = w\right).$$

Expand

$$\mathrm{e}^{\sum_{\ell=1}^{n}\sum_{I \supset Z(\ell)} \phi_\beta(|I|)} = \prod_\ell \prod_I \left((\mathrm{e}^{\phi_\beta(|I|)} - 1)\mathbb{1}_{Z(\ell)\in I} + 1\right)$$

and use resummation

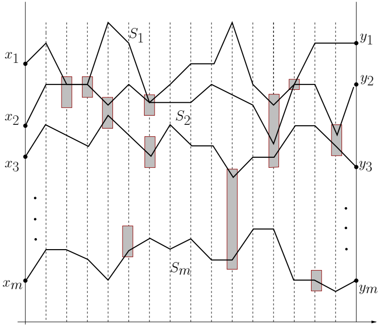
Attraction vrs Repulsion: m Walks

- Repulsion: $\mathcal{R}_n^+ = \{S_1(\ell) \geq S_2(\ell) \geq \cdots \geq S_m(\ell)\ \forall \ell = 0, 1, 2, \dots, n\}$

- Attraction: Via potential

$$\Phi_{\beta,n}(\underline{S}) = \sum_{\ell=1}^{n} \sum_{I \supset \underline{S}(\ell)} \phi_\beta(|I|) N(I, \underline{S}(\ell))$$

where, for an interval I and a tuple $\underline{x}$
$N(I, \underline{x}) = \max\{0, |I \cap \underline{x}| - 1\}$.



Lemma. For all β large enough

$$\log \mathbb{E}_{\underline{x}}\left(e^{\Phi_{\beta,n}(\underline{S})}; \mathcal{R}_n^+; \underline{S}(n) = \underline{y}\right) \lesssim m$$

uniformly in m, $\underline{x}, \underline{y}$ and $n \geq n_0$.

Attraction vrs Repulsion: m Walks

Remark: The case of SRW walks and one-point attractive potentials (only intersections are rewarded) was studied by Tanemura and Yoshida '03.

Proof in the General Case: For $\underline{z} = (z_1, z_2, \dots, z_m)$ ordered tuple and an interval I,

$$N(\underline{z}, I) = \sum_1^m \mathbb{1}_{\{(z_k, z_{k+1}) \in I\}} = \sum \mathbb{1}_{\{(z_{2k-1}, z_{2k}) \in I\}} + \sum \mathbb{1}_{\{(z_{2k}, z_{2k+1}) \in I\}}$$

On the other hand,

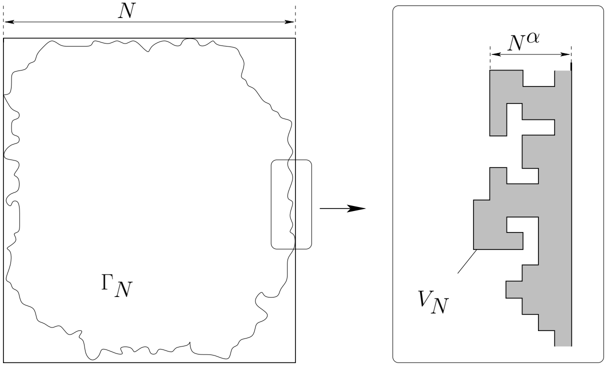
$$\mathcal{R}_n^+ \subset \left\{ \bigcap_k (S_{2k-1}(\cdot) \leq S_{2k}(\cdot)) \right\} \cap \left\{ \bigcap_k (S_{2k}(\cdot) \leq S_{2k+1}(\cdot)) \right\} \triangleq \mathcal{R}_n^{o,+} \cap \mathcal{R}_n^{e,+}$$

Use Cauchy-Swarz to decouple between even and odd constraints and then $m - 1$ times the upper bound for two walks.

Happy Birthday

Funaki-san !!!

Appendix: Fluctuations of (monolayer) boundaries



- Bulk fluctuation price for V_N is $\sim \frac{V_N N^2}{N^3} \sim \frac{V_N}{N}$.
- Repulsion price for staying N^α away from the boundary is $N^{1-2\alpha}$.

Therefore $N^{1-2\alpha} \sim \frac{V_N}{N} \sim \frac{N^{1+\alpha}}{N} = N^\alpha$ gives $\alpha = 1/3$.