Layering in the SOS Model Without External Fields

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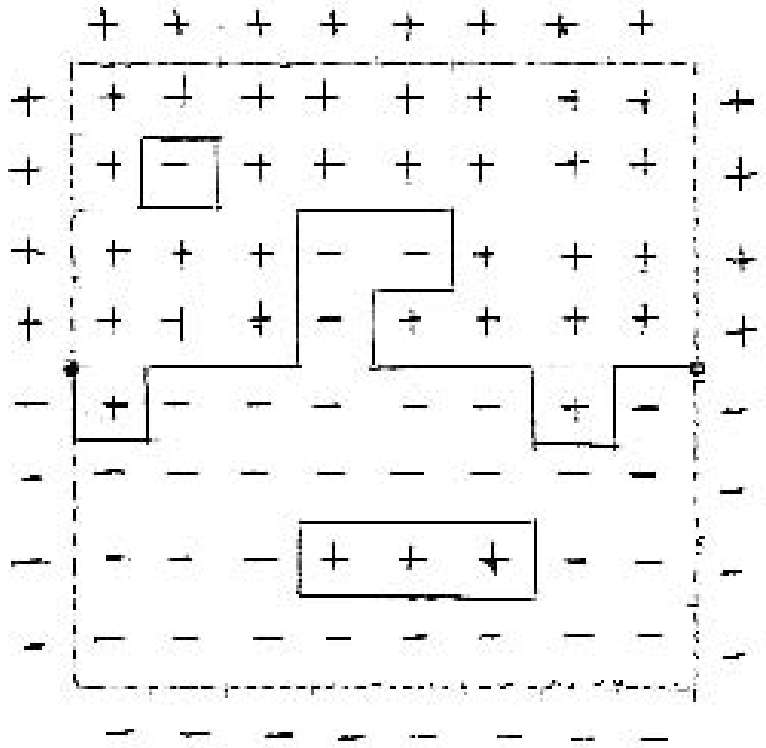
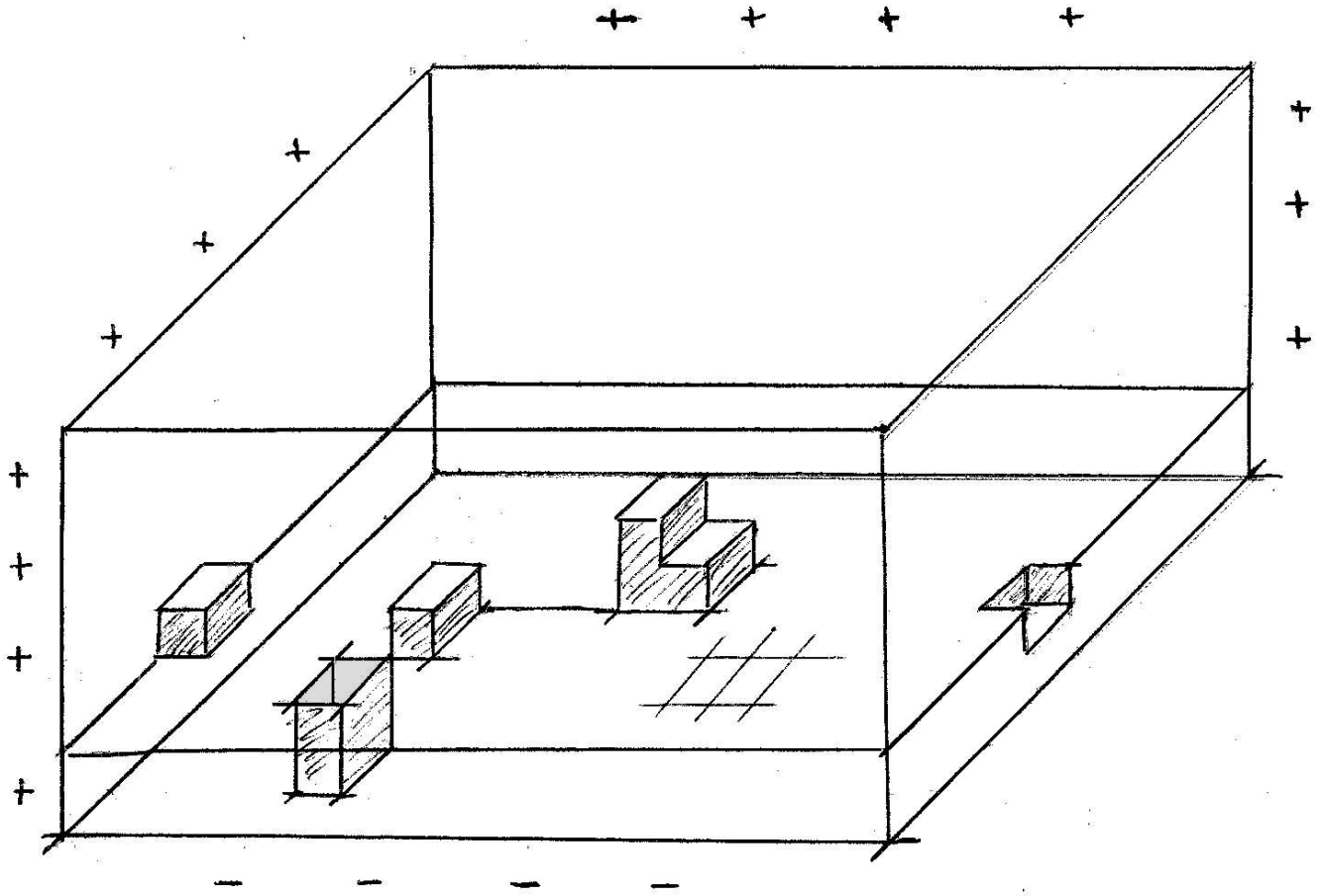
Start with the Ising model: Spin $\sigma_x = \pm 1$ at each site $x \in \Theta \subset \mathbb{Z}^d$, fixed boundary spins η, Hamiltonian (energy of configuration) given by

$$H(\sigma \mid \eta) = -J \sum_{\langle x,y \rangle} \sigma_x \sigma_y - h \sum_x \sigma_x, \quad \text{Boltzmann weight } e^{-\beta H(\sigma|\eta)},$$

where $\beta =$ inverse temperature. Put line segment separating each $\pm$ pair:



3d version: Ising model in a halfspace $\mathbb{Z}^2 \times \mathbb{Z}_+$, with a wall at height 0, below the critical temperature. Finite box $[-N, N]^2 \times [0, N]$ with minus boundary condition on the wall, plus boundary condition on the rest of the boundary. This forces the existence of an interface separating minus phase along the wall from the plus phase in the bulk.



At temperatures below the roughening temperature T_R (believed to be below T_c; recall $\beta = 1/T$), the interface will typically be flat, with height fluctuations of bounded order as $N \to \infty$.

Entropic repulsion will push the interface away from the wall: for a fixed interface height, the wall prevents certain fluctuations that would be possible in its absence. Hence ($h = 0$) interface height $\to \infty$ as $N \to \infty$.

To counter entropic repulsion:

(1) Add an external field $h > 0$. This favors the plus phase above the interface so effectively pushes the interface down. **OR:**

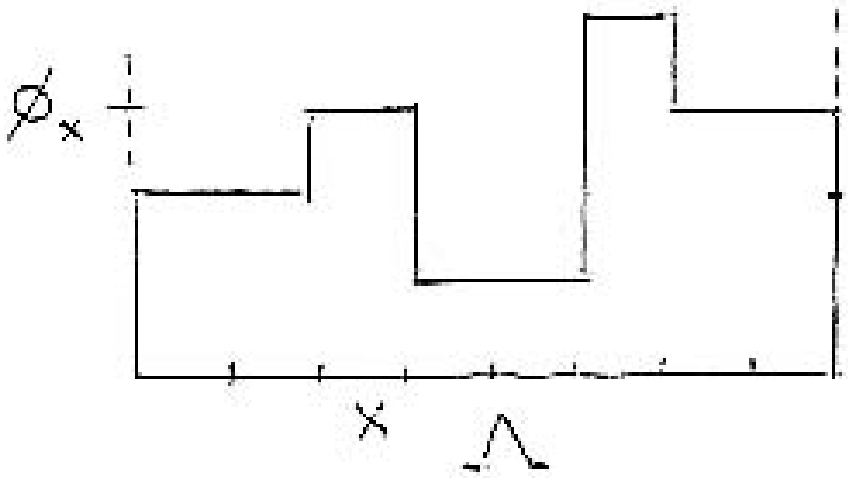
(2) Weaken the interaction with the wall: Ising interaction J in the bulk, interaction $K < J$ of bulk spin with a minus in the wall. Effectively, an energetic reward of $2(J - K)$ for each plaquette of the interface touching the wall. (0-field case.)

Solid-On-Solid (SOS) Approximation: Consider only the interface (ignore islands) and prohibit overhangs.

Region $\Lambda \subset \mathbb{Z}^2$, height ϕ_x at $x \in \Lambda$, boundary condition of height n outside Λ. For an interface $\mathcal{I}$ let $|\mathcal{I}|_v$ be the number of pairs of vertical plaquettes and $|\mathcal{I} \cap W|$ the number in contact with the wall. Hamiltonian for 0-field case:

$$H_\Lambda(\phi \mid n) = 4J|\mathcal{I}|_v - 2(J-K)|\mathcal{I} \cap W|.$$

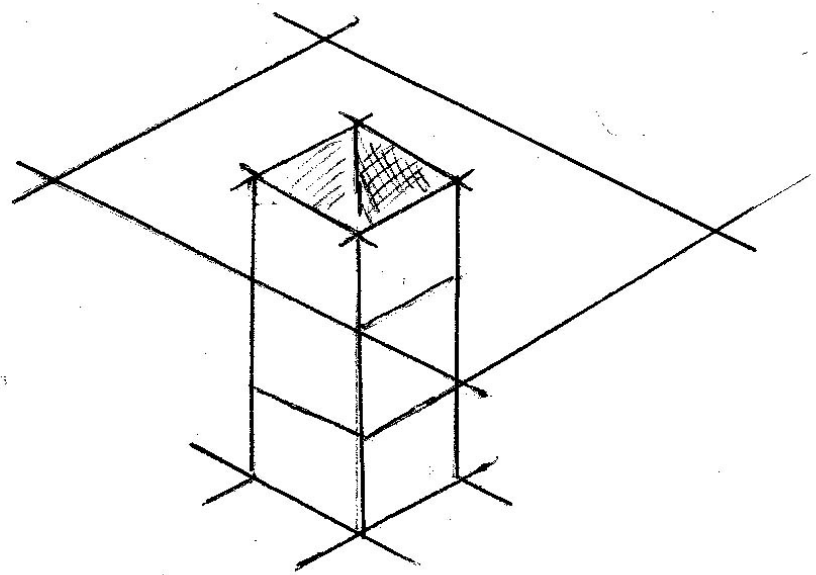
Note we don't count horizontal plaquettes, because there are always the same number $|\Lambda|$ of them.



For $t = e^{-4\beta J}$, $u = 2\beta(J - K)$, Boltzmann factor is

$$e^{-\beta H_\Lambda(\phi|n)} = e^{-4\beta J|\mathcal{I}|_v + 2\beta(J-K)|\mathcal{I}\cap W|} = t^{|\mathcal{I}|_v} e^{u|\mathcal{I}\cap W|}.$$

Each local perturbation contributes to the weight of the interface, e.g. $t^6 e^u$ for a $3 \times 1 \times 1$ column reaching the wall from height 3 (12 vertical plaquettes.) Low temperature $\leftrightarrow t \ll 1$. Consider $u \ll 1$ also.



Factor of t is the cost of 2 vertical plaquettes; u is the gain for each plaquette touching the wall. (Other horizontal plaquettes cancel out—fixed number of them.)

Substance A below the interface, substance B above. Possible phenomena:

Complete wetting: Interface height $\to \infty$ as $\Lambda \nearrow \mathbb{Z}^2$.

Partial wetting: Finite layer of A. There exists $n \geq 1$ such that the interface height is n (with high probability) for all sufficiently large Λ.

No wetting: Interface height 0 for sufficiently large Λ.

Layering: A sequence of transitions as the external field h or the wall attraction u is reduced, in which the equilibrium interface height steps $0 \to 1 \to 2 \to \cdots$. For each height n there is an interval of h or u values in which n is the equilibrium height, and at the transition point between n and $n+1$ there should be coexistence.

Known results:

Chalker (1982): (0-field) Complete wetting for small enough u, no wetting for large enough u.

Dinaburg and Mazel (1994): External field h, and β large. Layering occurs—there are a sequence of intervals of h values (with gaps between them) such that in the nth interval, where $h \approx \beta^{-1} e^{-4\beta n}$, the equilibrium height is n. Downward push of field balances entropic repulsion.

Cesi and Martinelli (1996): External field h, β large. Sharp transitions, with phase coexistence at the transition point, between height n and $n+1$, up to some height $n_{\max}(\beta)$ for which $n_{\max}(\beta) \to \infty$ as $\beta \to \infty$.

Lebowitz and Mazel (1996): Similar to Cesi and Martinelli, but for all n.

Ising version: Fröhlich and Pfister (1987), Basuev (2007)

Physics literature (mostly nonrigorous): Cahn (1977), Binder and Landau (1992)

Is there layering in the 0-field case?

ϕ_x = interface height at $x \in \mathbb{Z}^2$. Rewrite Hamiltonian as

$$\beta H_\Lambda(\phi \mid n) = \beta J \sum_{\langle x,y \rangle} |\phi_x - \phi_y| + \sum_x V(\phi_x),$$

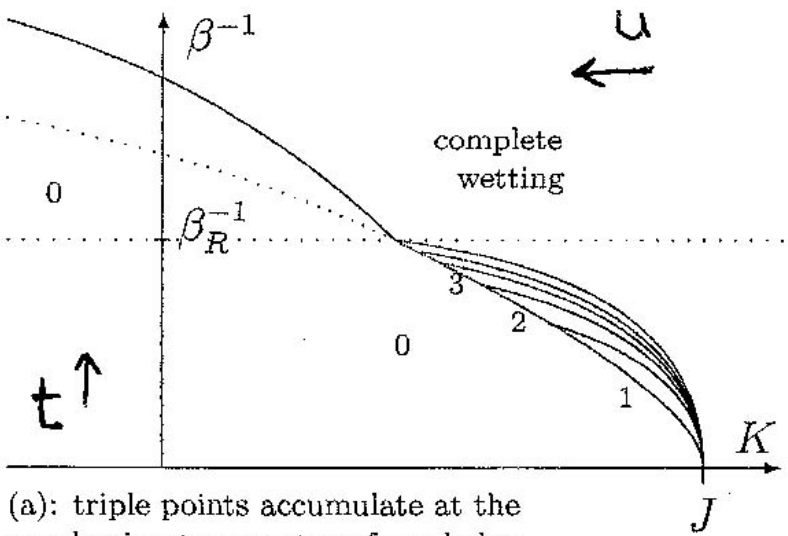
where

$$V(n) = \beta h n \quad \text{(external field case)},$$

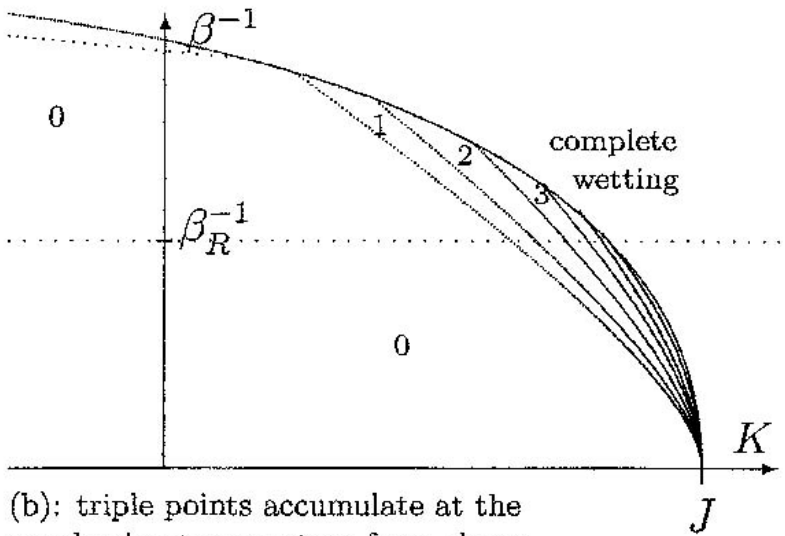
$$V(n) = \begin{cases} 0 & \text{if } n = 0 \\ u & \text{if } n \geq 1 \end{cases} \quad \text{(0-field case)}$$

Layering seems more "natural" when $V(n)$ increases to ∞: V overcomes entropic repulsion when interface exceeds some height. But is $V(n) \to \infty$ necessary for layering, or will it happen with the potential existing only at height 0?

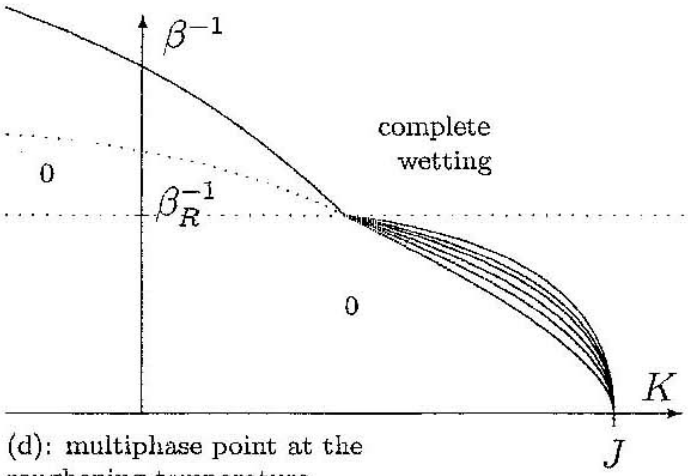
Physicists say yes, such layering will occur. But the phase diagram is poorly understood with multiple conflicting possibilities. Diagrams from Binder and Landau (1992)—recall $u = 2\beta(J - K)$ is the reward for touching the wall:



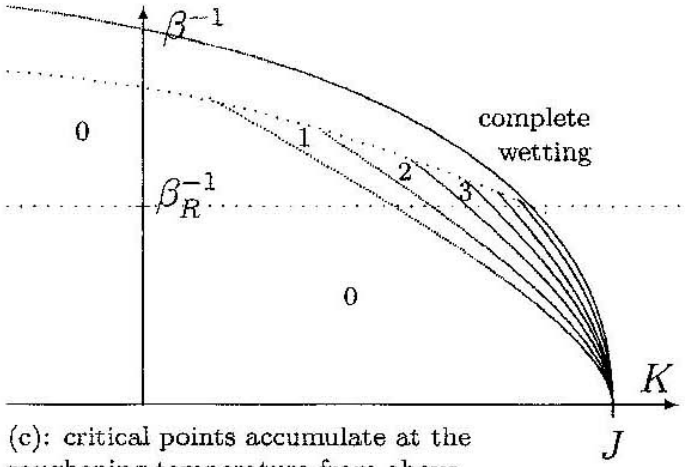
(a): triple points accumulate at the roughening temperature from below



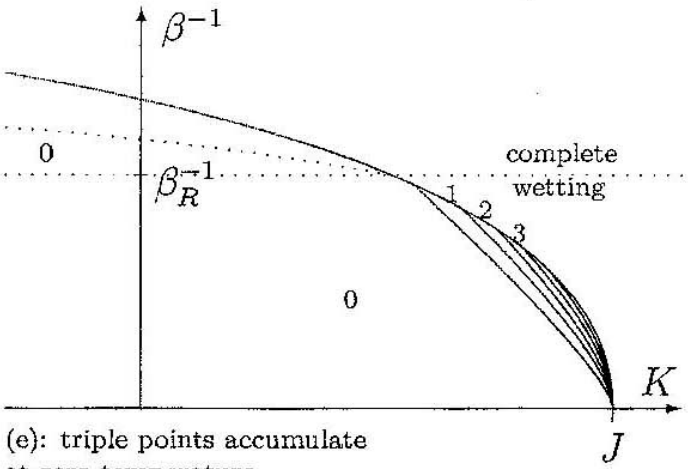
(b): triple points accumulate at the roughening temperature from above



(d): multiphase point at the roughening temperature



(c): critical points accumulate at the roughening temperature from above



(e): triple points accumulate at zero temperature

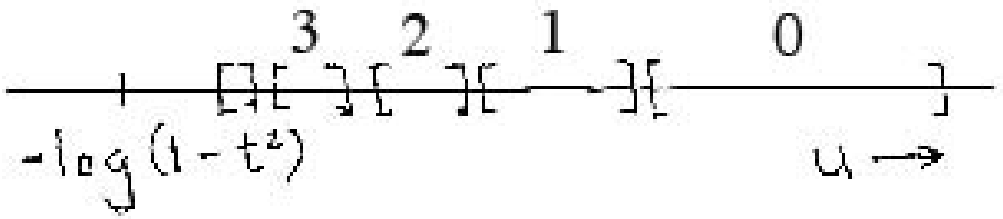
Rigorous result in the 0-field case

Layering does occur in 0-field case—critical value of u is near $-\log(1-t^2)+2t^{n+3}$ for transition from height n to $n+1$. (But we don't have proof of sharp transition—just intervals .) More precisely:

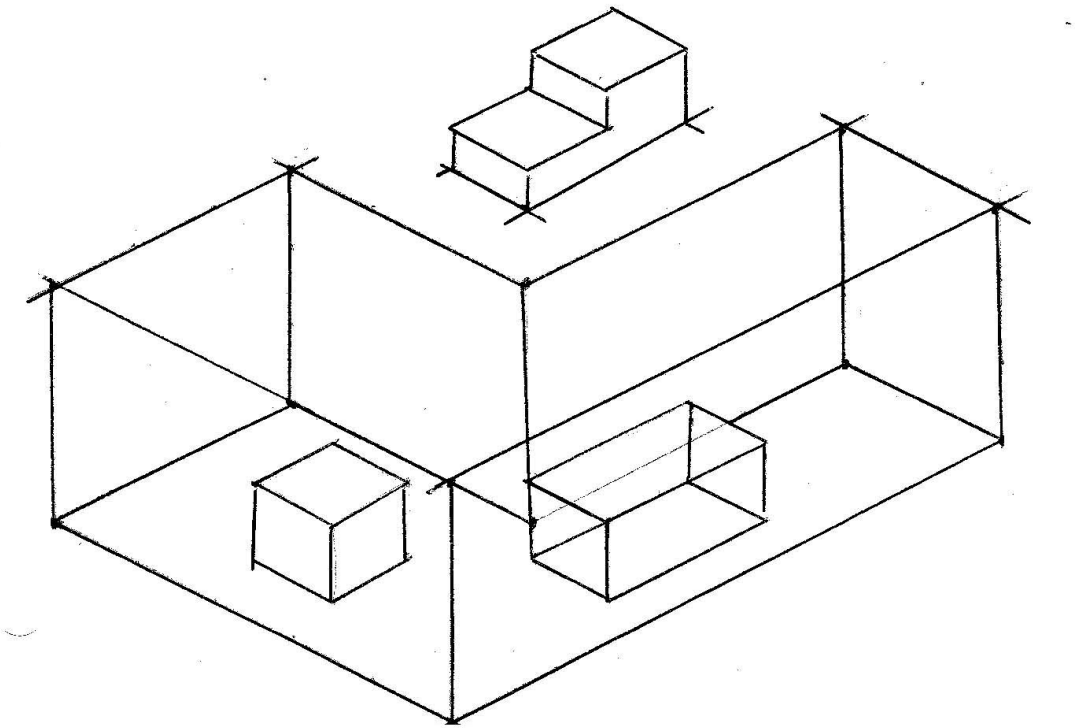
Theorem. (A., Dunlop, Miracle-Solé, 2011, JSP to appear) Fix a height $n \geq 0$, and $\epsilon > 0$. There exists $t_0(n,\epsilon)$ (of order n^{-4}) such that for $t < t_0$ and

$$u \in \begin{cases} [-\log(1-t^2)+(2+\epsilon)t^{n+3}, & \\ \quad -\log(1-t^2)+(2-\epsilon)t^{n+2}] & \text{if } n \geq 1, \\ [-\log(1-t^2)+(2+\epsilon)t^3, \sqrt{t}] & \text{if } n = 0, \end{cases}$$

(i) the cluster expansion in (t,u) converges, (ii) there is a unique translation-invariant Gibbs state, with the interface at height n, (iii) a positive fraction of horizontal plaquettes are in contact with the wall.



Proof Ideas: Height-n boundary condition outside region Λ, for some n. Then each configuration decomposes uniquely into *cylinders*:



Cylinder determined by its perimeter (a lattice loop) and its internal and external heights. Cylinder γ has weight $\varphi(\gamma) = t^m e^{ju}$ where m is the number of pairs of vertical plaquettes, and j is the (signed) number of horizontal plaquettes touching the wall.

Partition function for height-n boundary condition is

$$\Xi(\Lambda, n) = e^{u\delta_0(n)|\Lambda|} \sum_{\Gamma \in \mathcal{C}(\Lambda,n)} \prod_{\gamma \in \Gamma} \varphi(\gamma),$$

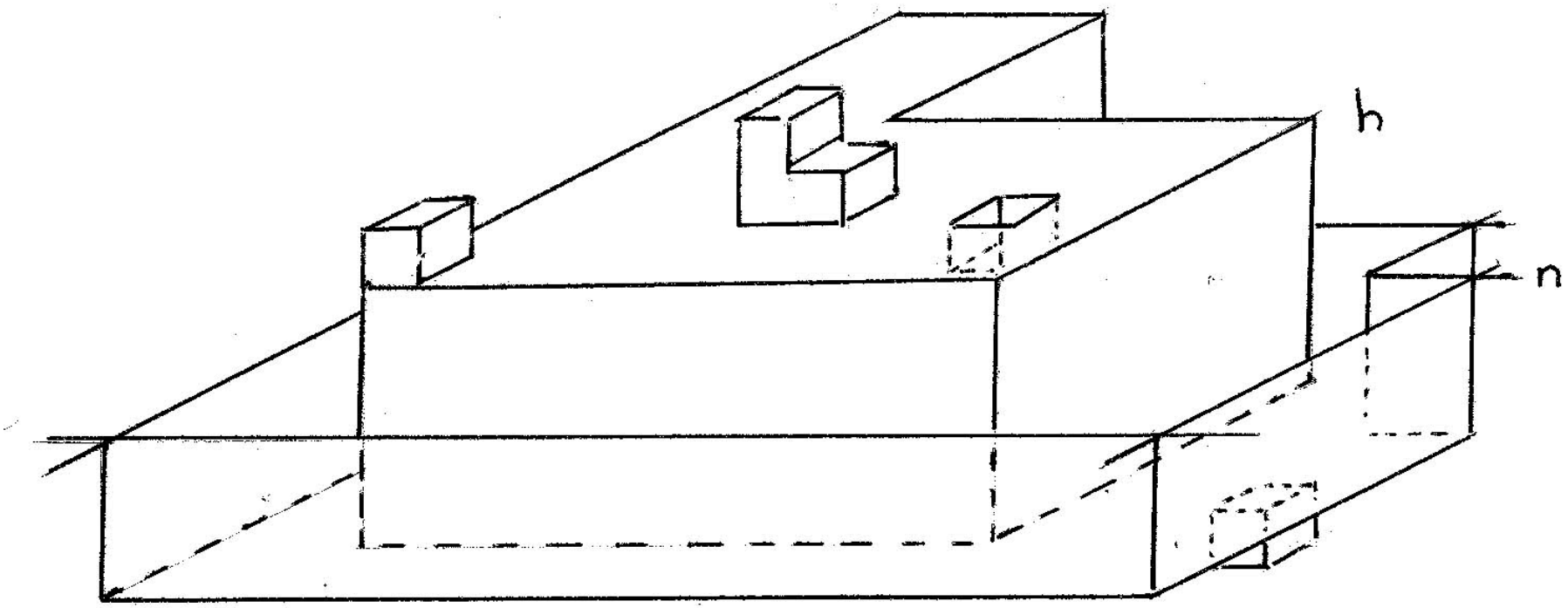
where $\mathcal{C}(\Lambda, n)$ is the set of all compatible collections of cylinders in Λ.

In a compatible collection Γ of cylinders, some are *external*, i.e. not inside any other cylinder.

A *perturbation* is a compatible collection with a unique external cylinder. The interface may be viewed as a flat surface interrupted by isolated perturbations.

Two types of cylinders according to size: let $k = \max(2n, 8)$. An *elementary cylinder* has diameter at most $3k + 3$. An *elementary perturbation* ω consists of only elementary cylinders. A *contour* Γ is a perturbation consisting of nonelementary cylinders (with certain restrictions.)

We want to view an interface as a collection of contours, augmented by elementary perturbations representing small local fluctuations.



Rewrite the partition function in terms of contours and elementary perturbations:

$$\Xi(\Lambda, n) = e^{u\delta_0(n)|\Lambda|} \sum_{\{\Gamma_i, \omega_j\}} \prod_i \varphi(\Gamma_i) \prod_j \varphi(\omega_j),$$

where for elementary perturbations ω, $\varphi(\omega)$ is just a product of the cylinder weights $\varphi(\gamma) = t^m e^{ju}$:

$$\varphi(\omega) = \prod_{\gamma \in \omega} \varphi(\gamma),$$

but for contours Γ it is not: Γ divides the support $\mathrm{Supp}(\Gamma)$ into regions R_i at heights h_i, and

$$\varphi(\Gamma) = \prod_{\gamma \in \Gamma} \varphi(\gamma) \frac{\prod_i Z_k^*(R_i, h_i)}{Z_k^*(\mathrm{Supp}(\Gamma), n)}.$$

The quotient on the right represents the effect on elementary perturbations from moving each region R_i from height n to h_i.

The partition functions in the quotient

$$\frac{\prod_i Z_k^*(R_i, h_i)}{Z_k^*(\mathrm{Supp}(\Gamma), n)}$$

correspond to *restricted ensembles*, which consist only of elementary perturbations. Here $n =$ interface height, $k = \max(2n, 8) =$ parameter defining "elementary" perturbations. Associated free energy

$$f_k(n) = -\lim_{\Lambda \nearrow \mathbb{Z}^2} \frac{1}{|\Lambda|} \log Z_k(\Lambda, n).$$

Idea: interface should prefer to be at the height n which minimizes $f_k(n)$. Then $f_k(h) - f_k(n)$ represents the cost per unit area for large regions at the "wrong" height h in a contour.

Cluster Expansion

Clusters X are collections of elementary perturbations (or contours) which are "connected by incompatibility relations," for example, $X = \{\omega_1, \omega_2, \omega_3, \omega_4\}$ with $\omega_1 \not\sim \omega_2, \omega_2 \not\sim \omega_3, \omega_2 \not\sim \omega_4$, where $\omega_i \not\sim \omega_j$ means the two are incompatible (cannot coexist in a configuration.)

Formal cluster expansion for the restricted ensemble:

$$f_k(h) = -u\delta(h) - \sum_{X\colon \operatorname{Supp} X \ni 0} \frac{1}{|\operatorname{Supp} X|} \varphi_u^T(X),$$

where

$$\varphi_u^T(X) = a^T(X) \prod_{\omega \in X} \varphi(\omega),$$

with $a^T(X)$ being a combinatorial factor related to inclusion-exclusion and Möbius functions. This is a power series in t with terms of form $ct^m e^{ju}$:

$$-f_k(h) = 1 + 2t^2 + 4t^3 - t^4 + \dots \qquad (\text{for } h \geq 2).$$

This restricted-ensemble cluster expansion is readily shown to converge for $t = O(k^{-4})$ and $u \le \sqrt{t}$, for all interface heights h. (Recall $k = \max(2n, 8)$.) We always tacitly assume such values of u, t.

For a given height n and sufficiently small t, can we choose the wall attraction u so that the free energy $f_k(h)$ is minimized at $h = n$?

Proposition. For $n \ge 1, \epsilon > 0$ and

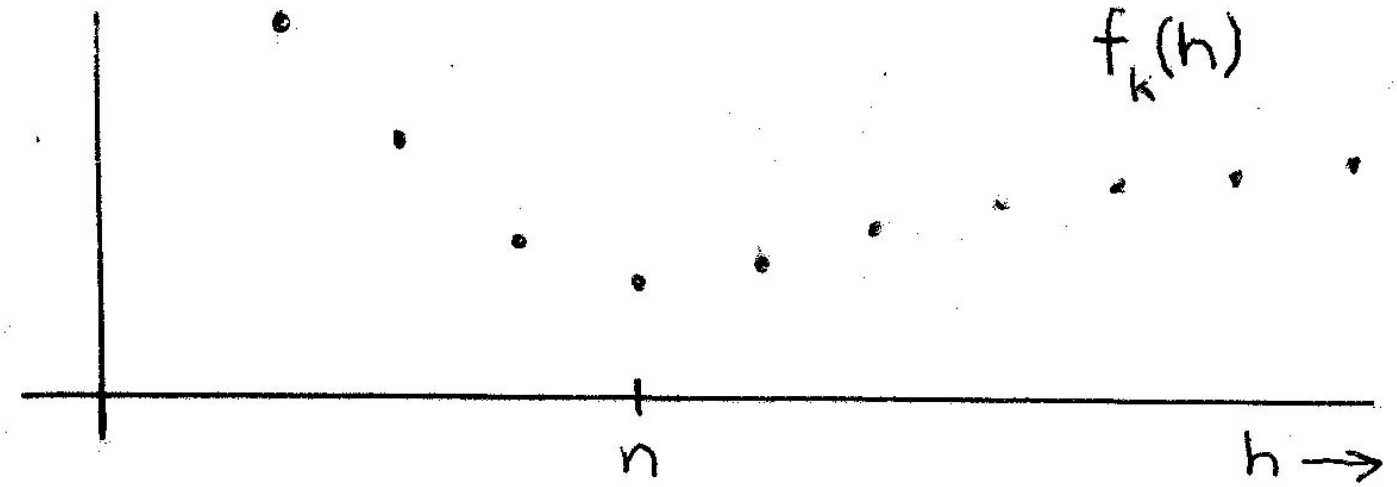
$$-\log(1-t^2) + (2+\epsilon)t^{n+3} \le u \le -\log(1-t^2) + (2-\epsilon)t^{n+2},$$

we have $f_k(h)$ minimized for $h = n$ (i.e. height n is *stable*):

$$\begin{aligned} f_k(h) - f_k(n) &\ge \epsilon t^{3n+3} + O(t^{3n+4}) \quad \text{for all } h \ge n+1, \\ f_k(h) - f_k(n) &\ge \epsilon t^{3h+3} + O(t^{3h+4}) \quad \text{for } h = n-1, \\ f_k(h) - f_k(n) &\ge 2t^{3h+3} + O(t^{3h+4}) \quad \text{for all } 0 \le h \le n-2. \end{aligned}$$

Key point–the hard part: the $O(\cdot)$ terms are *uniform in h and n*.

Uniformity in h and n ensures restricted free energy $f_k(h)$ is really minimized at height $h = n$:



Also, the requirement $t = O(k^{-4}) = O(n^{-4})$ means for fixed small t, we have heights $n = O(t^{-1/4})$ each stable in some interval, so the max stable height $\to \infty$ as $t \to 0$. But we cannot deal with heights $n \to \infty$ with a fixed t.

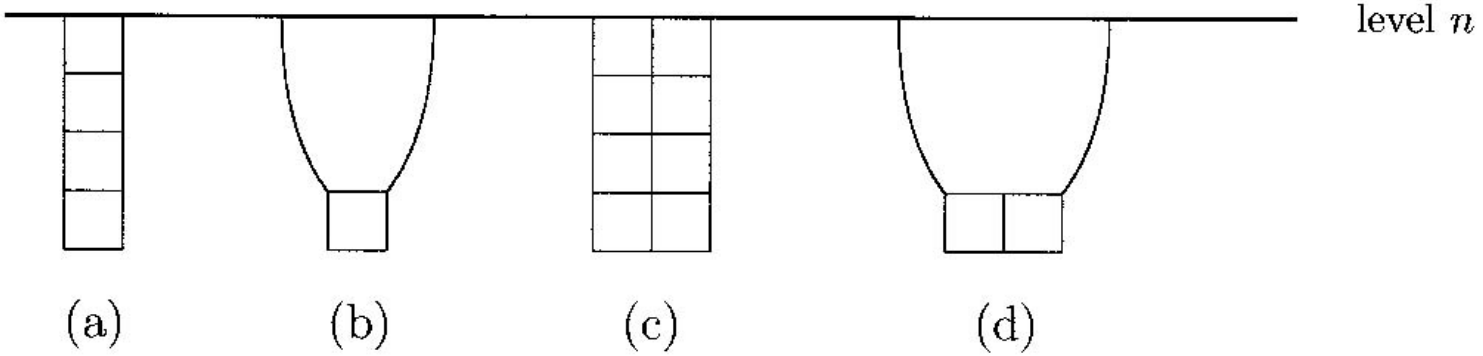
Open question: do we have a complete layering transition as $u \to 0$ (every height n stable in some interval of u values) for small t?

Dominant terms in the cluster expansion of $f_k(h+1) - f_k(h)$

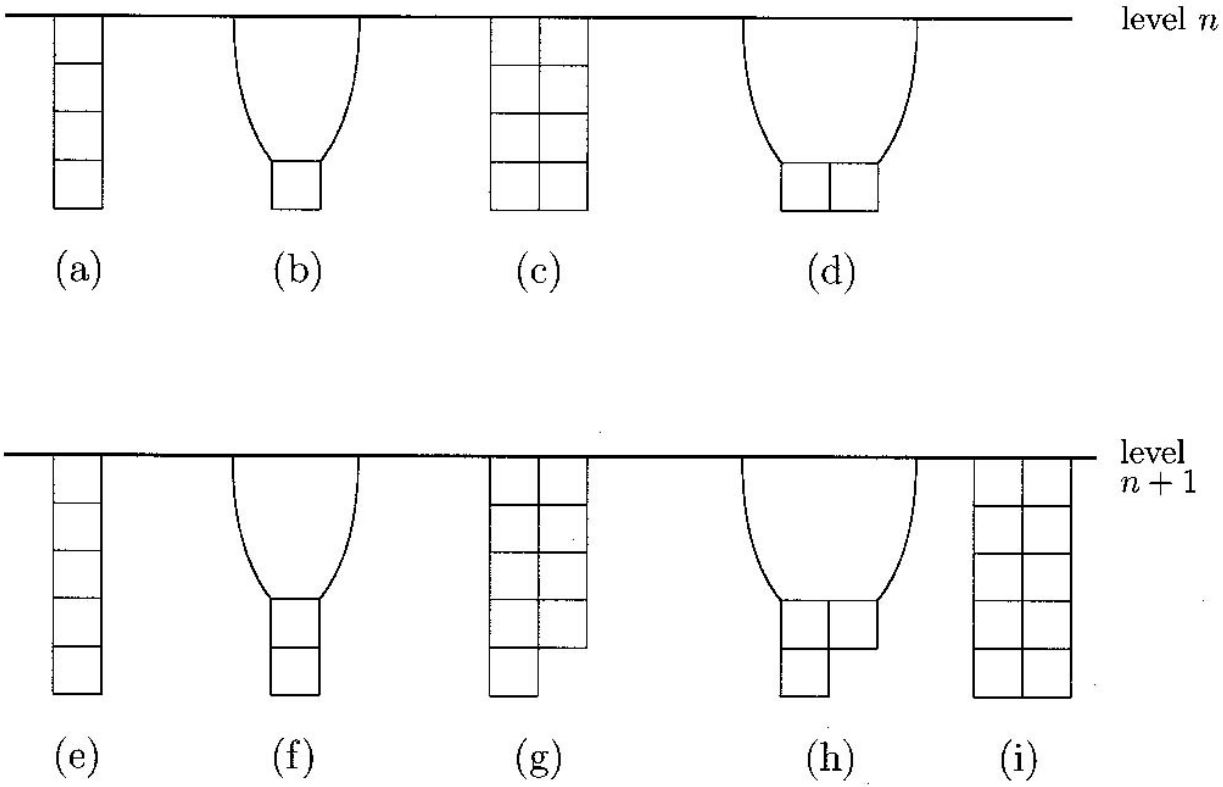
Dominant terms each $\leftrightarrow$ cluster which is a single elem. perturbation:

$$
\begin{aligned}
&f_k(h+1) - f_k(h) \\
&\quad = (t^{2h} + P_h(t))\big(e^u - 1 - t^2 e^u\big) + (2t^{3h} + Q_h(t))\big(e^{2u} - 1 - 2t^2 e^u\big) \\
&\qquad - 2t^{3h+3} e^{2u} + V_h(t,u),
\end{aligned}
$$

where $P_h(t) \leftrightarrow$ clusters of type (b), $Q_h(t) \leftrightarrow$ clusters of type (d), and $V_h(t,u) \leftrightarrow$ all types not shown. (More terms if $h \leq 3$.) Control of P_h, Q_h, V_h must be uniform in h. Here 2-d pictures represent 3-d objects:



There is a tradeoff between greater entropy (all of (a)–(i) can appear when interface is at height $n+1$, vs. only (a)–(d) at height n) and increased energy ((a)–(d) receive reward for touching the wall, when interface is at height n.) Where these balance should be the critical curve in (t, u) separating height-n phase from height-$(n+1)$ phase.



Main balance is (a), (e), (i); rest is smaller order (after cancellation.)

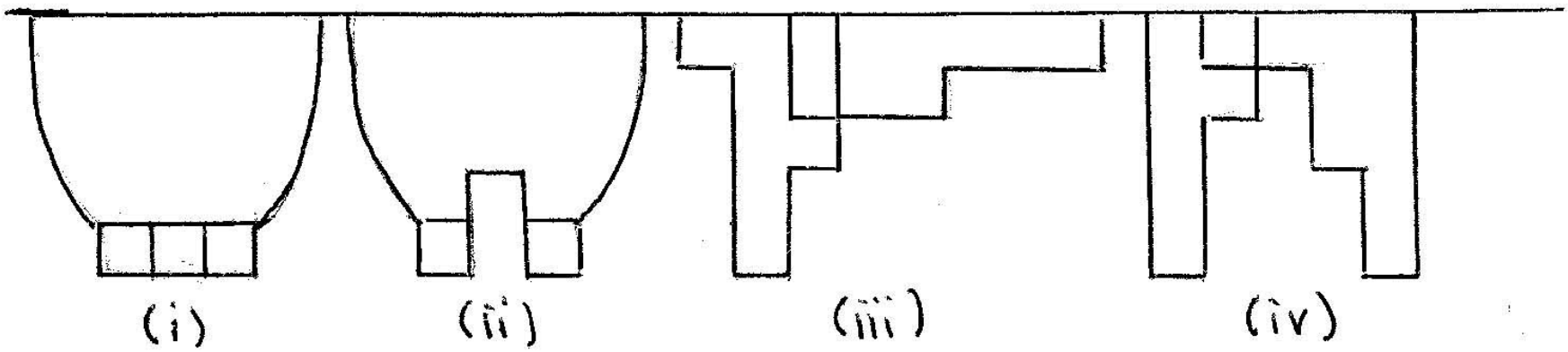
To prove the Proposition (i.e. to show $f_k(h)$ is minimized at $h = n$ in the appropriate interval of u values), we must control the "collected small terms" P_h, Q_h, V_h, uniformly in h. For V_h, we divide the terms (i.e. the clusters contributing to the sum) into types:

(i) Clusters in which some cylinder places 3 or more plaquettes on the wall;

(ii) Clusters in which there is an elementary perturbation in which two distinct cylinders place plaquettes on the wall;

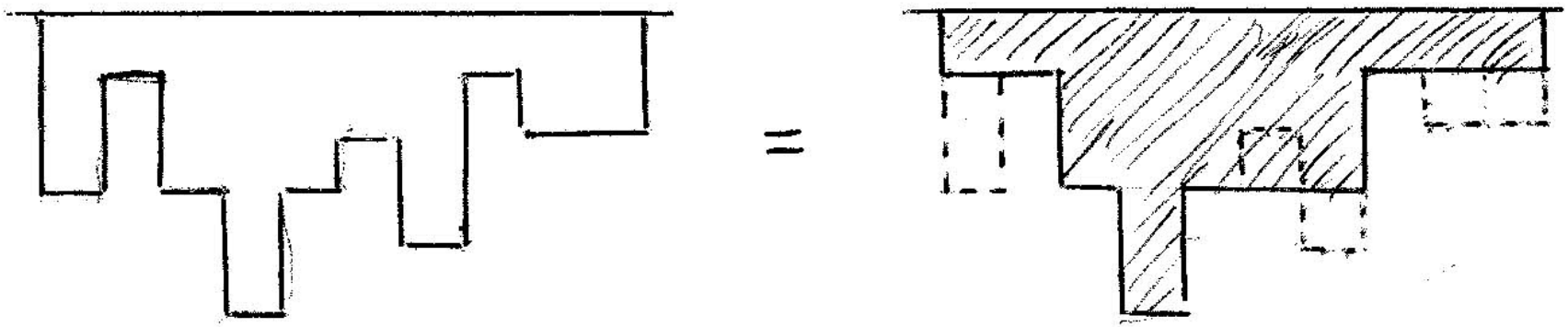
(iii) Clusters of large diameter which touch the wall;

(iv) Clusters in which two different elementary perturbations place plaquettes on the wall.

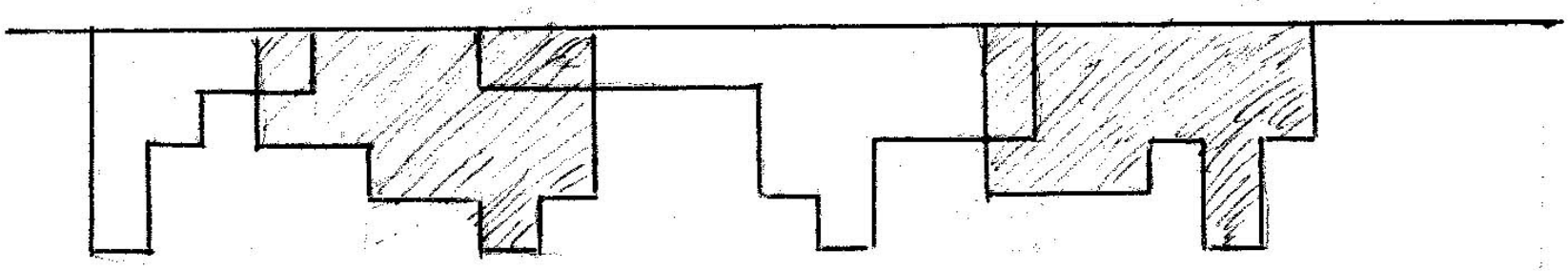


In summing the contribution from each type, we make use of:

(1) Structure of an elementary perturbation touching the wall: *tornado* (shaded) plus local fluctuations,



(2) Structure of the *incompatibility graph* of a cluster: vertices are the elementary perturbations, edges between incompatible pairs.



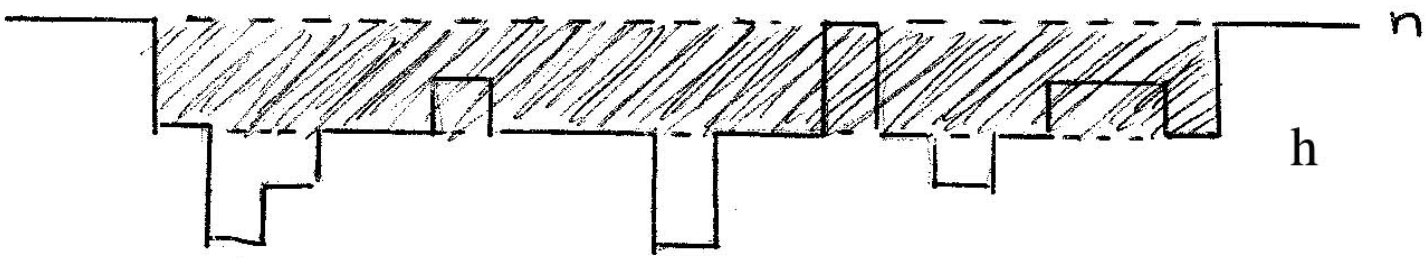
These 4 elementary perturbations correspond to a path in the graph.

The control we obtain on P_h, Q_h, V_h means they are negligible in the expression for the free energy increment:

$$\begin{aligned} & f_k(h+1) - f_k(h) \\ & \quad = (t^{2h} + P_h(t))\big(e^u - 1 - t^2 e^u\big) + (2t^{3h} + Q_h(t))\big(e^{2u} - 1 - 2t^2 e^u\big) \\ & \qquad - 2t^{3h+3} e^{2u} + V_h(t,u), \end{aligned}$$

which gives the desired minimization of $f_k(h)$ at interface height $h = n$ for our specified n, in the appropriate u interval. Proposition is proved.

To prove the Theorem, must make rigorous the idea that $f_k(h) - f_k(n)$ is the cost per unit area of placing a region R in a contour at height h. This ensures the interface "stays at height n except for local fluctuations."



Recall our earlier definition of the contour weight:

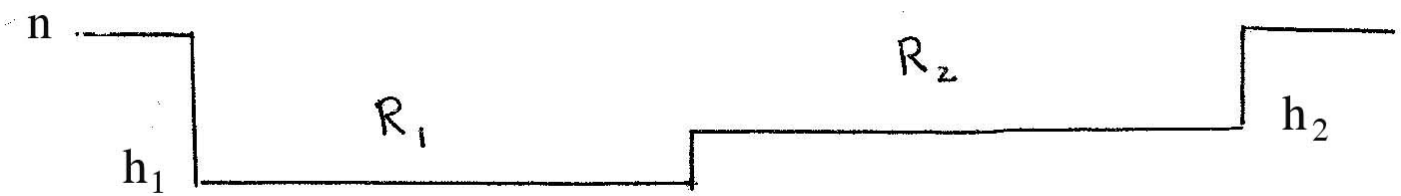
$$\varphi(\Gamma) = \prod_{\gamma \in \Gamma} \varphi(\gamma) \frac{\prod_i Z_k^*(R_i, h_i)}{Z_k^*(\mathrm{Supp}(\Gamma), n)},$$

where each R_i is a region of the contour at height h_i. Switch from Z_k^* to modified $\widehat{Z}_k$. Since $\mathrm{Supp}(\Gamma) = \cup_i R_i$ and boundaries reduce the partition function, we have

$$\widehat{Z}_k(\mathrm{Supp}(\Gamma), n) \geq \prod_i \widehat{Z}_k(R_i, n)$$

so we can treat each R_i separately:

$$\varphi(\Gamma) \leq \prod_{\gamma \in \Gamma} \varphi(\gamma) \prod_i \frac{\widehat{Z}_k(R_i, h_i)}{\widehat{Z}_k(R_i, n)},$$



We express these ratios as

$$\log \frac{\widehat{Z}_k(R_i, h_i)}{\widehat{Z}_k(R_i, n)} = -|R_i|(f_k(h_i) - f_k(n)) + \text{“boundary terms”},$$

describe exactly what the boundary terms are, and bound them (similar to bounding the full restricted-ensemble cluster expansion, when we show it converges.) Result is that in the desired interval for height $n \geq 1$:

$$u \in [-\log(1 - t^2) + (2 + \epsilon)t^{n+3}, -\log(1 - t^2) + (2 - \epsilon)t^{n+2}],$$

we have for $h \neq n$:

$$\frac{\widehat{Z}_k(R_i, h_i)}{\widehat{Z}_k(R_i, n)} \leq \exp\left(-\frac{\epsilon}{2}|R_i|t^{3n+3} + K|\partial R_i|t^2\right),$$

meaning there is a cost at least of order t^{3n+3} per unit area for having region R_i at the “wrong height” $h_i \neq n$.

We can use this to bound the cluster weight $\varphi(\Gamma)$ by something we will show is summable over clusters:

$$\begin{aligned}\varphi(\Gamma) &\le \left(\prod_{\gamma\in\Gamma}\varphi(\gamma)\right)\prod_i \frac{\widehat{Z}_k(R_i,h_i)}{\widehat{Z}_k(R_i,n)} \\ &\le \left(\prod_{\gamma\in\Gamma}\varphi(\gamma)\right)\exp\left(-\sum_i \frac{\epsilon}{2}|R_i|t^{3n+3}+\sum_i K|\partial R_i|t^2\right).\end{aligned}$$

Each boundary ∂R_i is composed of pieces of perimeters of the cylinders γ, so the cylinder weights $\prod_{\gamma\in\Gamma}\varphi(\gamma)$ more than cancel the positive term $\sum_i K|\partial R_i|t^2$ in the exponent.

We fix n and consider clusters of perturbations with external height n, with u in the appropriate interval to make n optimal. To show that we really do have a stable interface at height n (i.e. only local fluctuations, with only $O(t^2)$ fraction of sites not at height n) the main thing is to show the cluster expansion of the surface tension converges—essentially, the contour weights that we just bounded can be summed. The formal cluster expansion of the surface tension is (summing over clusters X)

$$\tau = -\frac{u}{\beta}\delta_0(n) - \frac{1}{\beta}\sum_{\text{Supp}\, X \ni 0} \frac{1}{|\,\text{Supp}\, X|}\varphi_u^T(X),$$

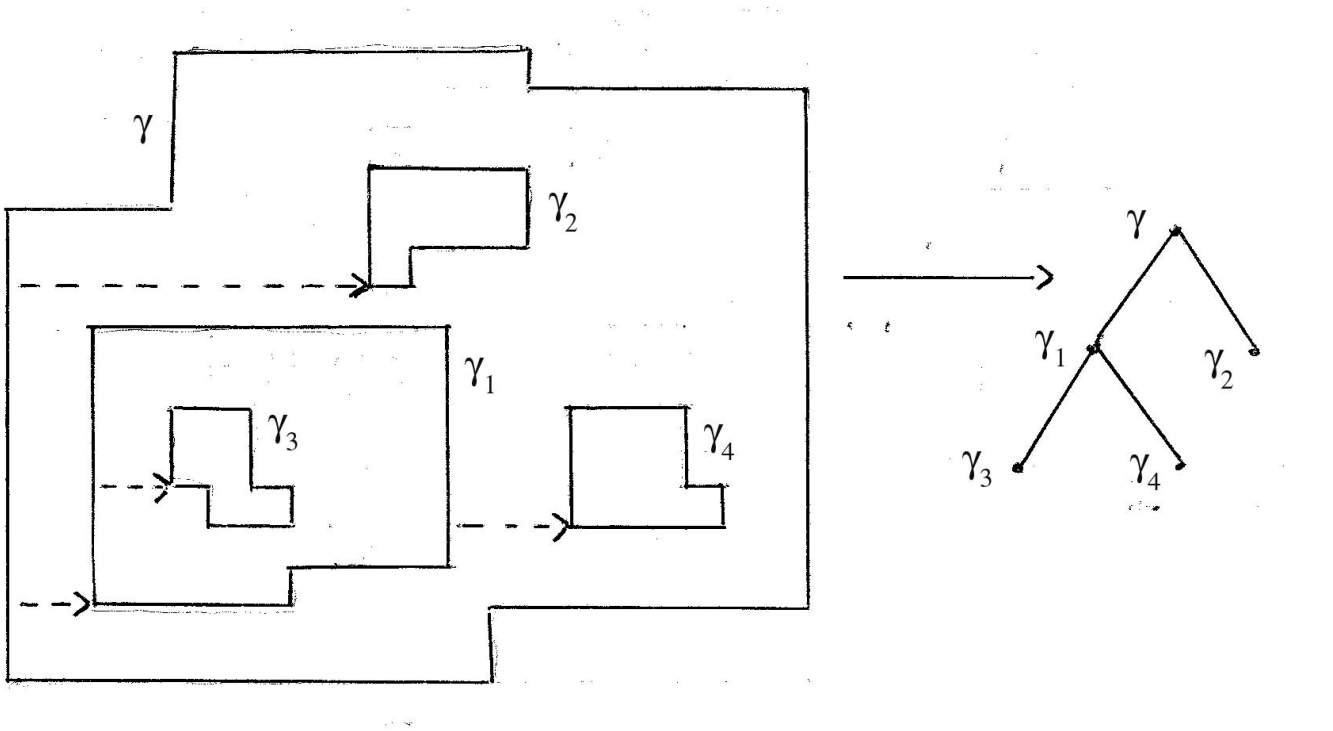
and by standard theory this converges if we show that for slightly larger contour weights $\mu(\Gamma) \geq \varphi(\Gamma)$ we have

$$\sum_{\Gamma:\text{Supp}(\Gamma)\ni 0} \mu(\Gamma) \leq (16t)^{3k+4}.$$

(Recall $k = \max(2n, 8)$.) Note the last sum is over contours not clusters.

We now have a weight $\varphi(\Gamma)$ (or its bound $\mu(\Gamma)$) which decreases exponentially in the contour area, and also in the total perimeter of all cylinders. How do we sum this over contours? Modify an idea from Dinaburg and Mazel (1994).

Contour (top view here) maps to a rooted tree with labeled edges and vertices:



Vertex label = perimeter length, edge label = length of dotted arrow.

Total of edge weights in the tree is at most the area $|\mathrm{Supp}(\Gamma)|$, since dotted arrows are disjoint.

We can sum over the rooted weighted trees to bound the sum of contour weights:

$$\sum_{\Gamma:\mathrm{Supp}(\Gamma)\ni 0} \mu(\Gamma) \le (16t)^{3k+4}.$$

Convergence of the cluster expansion is established, and the sum is $O(t^2)$ which shows that (in the appropriate interval of u values) the fraction of locations with heights $\neq n$ is $O(t^2)$, meaning the interface truly is at height n.