MATHEMATICS OF PHASE TRANSITIONS

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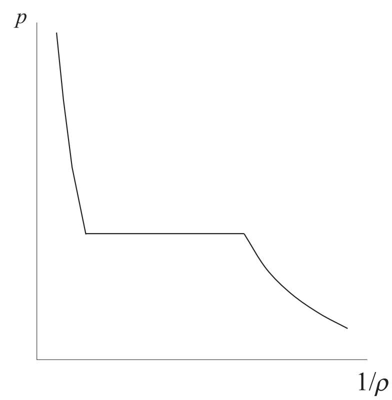
Abstract: This is a very brief introduction to the theory of phase transitions. Only few topics are chosen with a view on possible connection with discrete mathematics. Cluster expansion theorem is presented with a full proof. Finite-size asymptotics and locations of zeros of partition functions are discussed among its applications to simplest lattice models. A link with the study of zeros of the chromatic polynomial as well as the Lovász local lemma is mentioned.

A prototype of a phase transitions is liquid-gas evaporation. With increasing pressure p (at a fixed temperature), the density ρ abruptly increases:

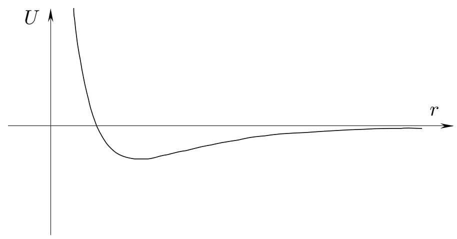


Follow Gibbs's precription: start from microscopic energy of the gas of N particles

$$H_N(\vec{p}_1, \dots, \vec{p}_N, \vec{r}_1, \dots, \vec{r}_N) = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i,j=1}^{N} U(\vec{r}_i - \vec{r}_j), \tag{1}$$

with interaction, for realistic gases, something like the Lenard-Jones potential, $U(r) \sim -\left(\frac{\alpha}{r}\right)^6 + \left(\frac{\alpha}{r}\right)^{12}$, with strong short range repulsion and long range attraction,

These are *lecture notes*: an edited version of lectures' transparencies. As a result, some topics are treated rather tersely and the reader should consult the cited literature for a more detailed information.



Basic thermodynamic quantities are then given in terms of
grand-canonical partition function

$$\begin{aligned} Z(\beta,\lambda,V) &= \sum_{N=0}^{\infty} \frac{z^N}{N!} \int_{\mathbb{R}^{3N}\times V^N} e^{-\beta H_N} \frac{\prod d^3\vec{p}_i \prod d^3\vec{r}_i}{h^{3N}} = \\ &= \sum_{N=0}^{\infty} \frac{\lambda^N}{N!} \int_{V^N} e^{-\beta\sum_{i,j} \Phi(\vec{r}_i-\vec{r}_j)} \prod d^3\vec{r}_i. \end{aligned} \tag{2}$$

Namely, for a given inverse temperature $\beta = \frac{1}{kT}$ and fugacity λ, the pressure is

$$p(\beta,\lambda) = \frac{1}{\beta} \lim_{V\to\infty} \frac{1}{|V|} \log Z(\beta,\lambda,V) \tag{3}$$

and the density

$$\rho(\beta,\lambda) = \lim_{V\to\infty} \frac{1}{|V|} \lambda \frac{\partial}{\partial\lambda} \log Z(\beta,\lambda,V). \tag{4}$$

However, to really prove the existence of gas-liquid phase transition along these lines remains till today an open problem. One can formulate it as follows:

Prove that for β large there exists $\lambda_t(\beta)$ such that $\rho(\beta,\lambda)$ is discontinuous at λ_t.

Much more is known and understood for *lattice models*, with Ising model as the simplest representative.

1. Ising model

For $x \in \mathbb{Z}^d$ take $\sigma_x \in \{-1,+1\}$ and using σ_Λ to denote $\sigma_\Lambda = \{\sigma_x; x\in\Lambda\}$ for any finite $\Lambda \subset \mathbb{Z}^d$, we introduce the energy

$$H(\sigma_\Lambda) = -\sum_{\langle x,y\rangle\subset\Lambda} \sigma_x\sigma_y - h\sum_{x\in\Lambda}\sigma_x.$$

The ground states (with minimal energy) for $h=0$ are the configurations $\sigma_\Lambda = \underline{+1}$, $\sigma_\Lambda = \underline{-1}$.

At nonzero temperature one considers the Gibbs state, i.e. the probability distribution:

$$\langle f\rangle_\Lambda^{\beta,h} = \frac{1}{Z_\Lambda(b,h)} \sum_{\sigma_\Lambda} f(\sigma_\Lambda) e^{-\beta H(\sigma_\Lambda)},$$

where

$$Z_\Lambda(\beta, h) = \sum_{\sigma_\Lambda} e^{-\beta H(\sigma_\Lambda)}.$$

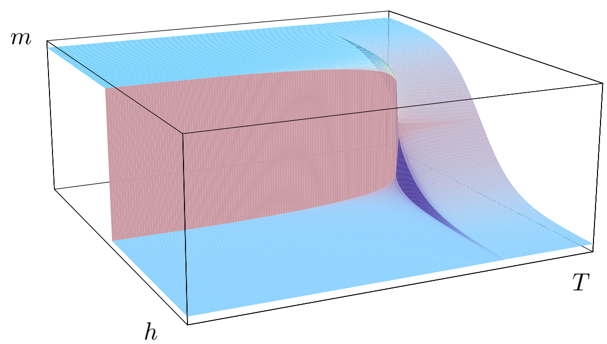
Phase transition are discussed in terms of the *free energy*

$$f(\beta, h) = -\frac{1}{\beta}\frac{1}{|\Lambda|}\lim_{\Lambda\nearrow\mathbb{Z}^d} \log Z_\Lambda(\beta, h)$$

and the *order parameter*

$$m(\beta, h) = \lim_{\Lambda\nearrow\mathbb{Z}^d} \langle \frac{1}{|\Lambda|}\sum_{x\in\Lambda} \sigma_x \rangle_\Lambda^{\beta,h}$$

that is should feature a discontinuity at low temperatures and $h = 0$:



Notice:

- $m(\beta, h) = -\frac{\partial f(\beta,h)}{\partial h}$ whenever f is differentiable,
- f is a concave function of h.

Define *spontaneous magnetization*: $m^*(\beta) = \lim_{h\to 0+} m(\beta, h)$.

An alternative formulation of the discontinuity is in terms of nonstability with respect to boundary conditions (up to now we have actually used *free boundary conditions*).

Given a configuration $\bar{\sigma}$, take

$$H_\Lambda(\sigma_\Lambda \mid \bar{\sigma}) = H(\sigma_\Lambda) - \sum_{x\in\Lambda, y\notin\Lambda} \sigma_x \bar{\sigma}_y$$

and, correspondingly,

$$\langle \cdot \rangle_{\Lambda,\bar{\sigma}}^{\beta,h} \quad \text{and} \quad Z_{\Lambda,\bar{\sigma}}(\beta, h).$$

Rather straightforward claims:

- f does not depend on $\bar{\sigma}$:

$$f(\beta, h) = -\frac{1}{\beta}\frac{1}{|\Lambda|}\lim_{\Lambda\nearrow\mathbb{Z}^d} \log Z_{\Lambda,\bar{\sigma}}(\beta, h)$$

- $m_{\bar\sigma}(\beta,h)=\lim_{\Lambda\nearrow\mathbb{Z}^d}\langle\frac{1}{|\Lambda|}\sum_{x\in\Lambda}\sigma_x\rangle^{\beta,h}_{\Lambda,\bar\sigma}$ may depend on $\bar\sigma$. Actually,

$$\boxed{m^*(\beta)=m_+(\beta,0)=\lim_{\Lambda\nearrow\mathbb{Z}^d}\langle\sigma_x\rangle^{\beta,h}_{\Lambda,+}}$$

Idea of the proof:

- $-\partial_h^- f(\beta,h)\le m_{\bar\sigma}(\beta,h)\le -\partial_h^+ f(\beta,h)$,
- $\lim_{h\to 0+} m_{\bar\sigma}(\beta,h)=-\partial_h^+ f(\beta,0)$ does not depend on the boundary condition,
- monotonicity of $\langle\frac{1}{|\Lambda|}\sum_{x\in\Lambda}\sigma_x\rangle^{\beta,h}_{\Lambda,+}$ on Λ, h,

$$\lim_{h\to0+}\lim_{\Lambda}=\inf_{h\ge0}\inf_{\Lambda}=\inf_{\Lambda}\inf_{h\ge0}=m_+(\beta,0).$$

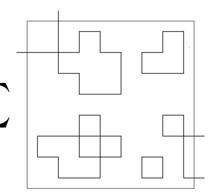
For **high temperatures**, the spontaneous magnetization vanishes,

$$\boxed{\tanh\beta<\tfrac{1}{2d-1}\implies m_+(\beta,0)=0.}$$

Proof: Expand $\prod_{\langle x,y\rangle\in E(\Lambda)}e^{\beta\sigma_x\sigma_y}$ with the help of

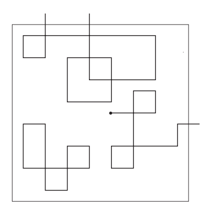
$$e^{\beta\sigma_x\sigma_y}=\cosh\beta\big(1+\sigma_x\sigma_y\tanh\beta\big).$$

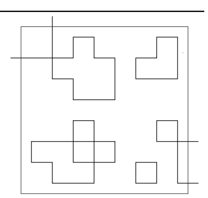
$$Z_{\Lambda,+}=\big(\cosh\beta\big)^{|E(\Lambda)|}\sum_{\sigma_\Lambda}\sum_{E\subset E(\Lambda)}\prod_{\langle x,y\rangle\in E}\big(\sigma_x\sigma_y\tanh\beta\big)=$$

$$=2^{|\Lambda|}\big(\cosh\beta\big)^{|E(\Lambda)|}\sum_{E\subset E(\Lambda)}\big(\tanh\beta\big)^{|E|}=2^{|\Lambda|}\big(\cosh\beta\big)^{|E(\Lambda)|}\sum$$ 

As a result,

$$\langle\sigma_x\rangle_{\Lambda,+}=\frac{\sum \text{[figure 2]}}{\sum \text{[figure 3]}}\le\sum_{\omega:x\to\partial\Lambda}\big(\tanh\beta\big)^{|\omega|}\le\sum_{n=\mathrm{dist}(x,\partial\Lambda)}^{\infty}(2d-1)^n\big(\tanh\beta\big)^n\to0.$$





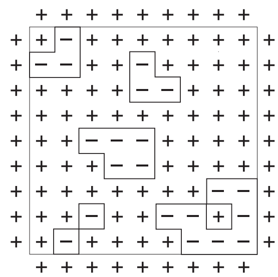
□

On the other hand, for **low temperatures**, there is a non-vanishing spontaneous magnetisation,

$$\boxed{d \geq 2, \exists \beta_0 : \beta \geq \beta_0 \implies m_+(\beta, 0) > 0.}$$

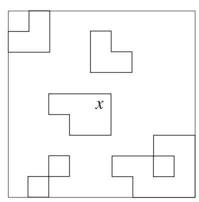
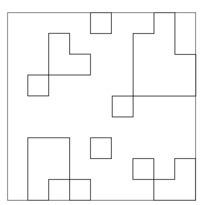
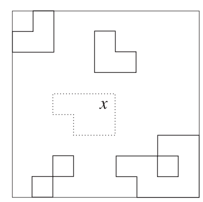
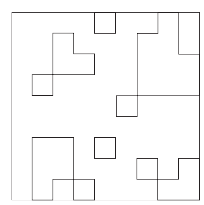
Proof: This is the famous Peierls argument:

Start with contour representation, $\sigma_\Lambda \longleftrightarrow \Gamma = \{\gamma_1, \gamma_2, \dots\}$:



It yields $H(\sigma_\Lambda \mid +) - \underbrace{H(+ \mid +)}_{E(\Lambda)} = 2 \sum_{\gamma \in \Gamma} |\gamma|$ and thus $Z_{\Lambda,+}(\beta, 0) = e^{\beta E(\Lambda)} \sum_{\Gamma \text{ in } \Lambda} e^{-2\beta \sum_{\gamma \in \Gamma} |\gamma|}$.

Writing $\langle \sigma_x \rangle_{\Lambda,+}^{\beta,0} = P_{\Lambda,+}(\sigma_x = 1) - P_{\Lambda,+}(\sigma_x = -1) = 1 - 2P_{\Lambda,+}(\sigma_x = -1)$, we evaluate

$P_{\Lambda,+}(\sigma_x = -1) \leq$ $\dfrac{\sum}{\sum}$ (numerator: $\sum$ ; denominator: $\sum$ ) $\leq \sum_{\gamma \text{ surr. } x} e^{-2\beta|\gamma|}$ $\dfrac{\sum}{\sum}$ (numerator: $\sum$ ; denominator: $\sum$ ) $\leq \sum_{k=4}^{\infty} e^{-2\beta k} \dfrac{k}{2} 3^{2(k-1)}$

using that $\#\{\gamma \text{ surrounds } x \mid |\gamma| = k\}$ is (for $d = 2$) bounded by $\frac{k}{2} 3^{2(k-1)}$. $\square$

Analysing the proof: 2 main ingrediences:

- *Independence of contours* (taking away any one (by flipping all spins inside it), what remains is still a valid configuration).
- *Damping* ($e^{-2\beta|\gamma|}$ is small for β large).

We met two expansions:

$$\sum_F \prod_{g \in F} \big(\tanh \beta\big)^{|g|} \qquad \text{and} \qquad \sum_\Gamma \prod_{\gamma \in \Gamma} e^{-2\beta|\gamma|}$$

(in the first sum we view the set $E \subset E(\Lambda)$ as a collection F of its connected components—high temperature polymers). Both expressions have the same structure of a sum over collections of pairwise independent contributions. This is a starting point of an abstract theory of cluster expansions. Its mature formulation is best presented as a claim about graphs with weights attributed to their vertices and I cannot resist presenting its full proof as it was substantially simplified in recent years [Dob96, SS05, M-Sol00, U04].

2. Cluster expansions

Consider:
A *graph* $G = (V, E)$ (without selfloops), and a *weight* $w : V \to \mathbb{C}$.
The term *abstract polymers* is also used for vertices $v \in V$, with pairs $(v, v') \in E$ being called *incompatible* (no sefloops: only distinct vertices may be incompatible).
For $L \subset V$, we use $G[L]$ to denote the induced subgraph of G spanned by L.

For any finite $L \subset V$, define

$$Z_L(w) = \sum_{I \subset L} \prod_{v \in I} w(v). \tag{5}$$

with the sum running over all *independent sets* I of vertices in L (no two vertices in I are connected by an edge). In other words: the sum is over all collections I of compatible abstract polymers.

The partition function $Z_L(w)$ is an entire function in $w = \{w(v)\}_{v \in L} \in \mathbb{C}^{|L|}$ and $Z_L(0) = 1$. Hence, it is nonvanishing in some neighbourhood of the origin $w = 0$ and its logarithm is, on this neighbourhood, an analytic function yielding a convergent Taylor series

$$\log Z_L(w) = \sum_{X \in \mathcal{X}(L)} a_L(X) w^X. \tag{6}$$

Here, $\mathcal{X}(L)$ is the set of all multi-indices $X : L \to \{0, 1, \dots\}$ and $w^X = \prod_v w(v)^{X(v)}$. Inspecting the Taylor formula for $a_L(X)$ in terms of corresponding derivatives of $\log Z_L(w)$ at the origin $w = 0$, it is easy to show that the coefficients $a_L(X)$ actually do not depend on L: $a_L(X) = a_{\operatorname{supp} X}(X)$, where $\operatorname{supp} X = \{v \in V : X(v) \neq 0\}$. As a result, one is getting the existence of coefficients $a(X)$ for each $X \in \mathcal{X} = \{X : V \to \{0, 1, \dots\}, |X| = \sum_{v \in V} |X(v)| < \infty\}$ such that

$$\log Z_L(w) = \sum_{X \in \mathcal{X}(L)} a(X) w^X \tag{7}$$

for every finite $L \subset V$ (convergence on a small neighbourhood of the origin depending on L).

Notice that $a(X) \in \mathbb{R}$ for all X (consider $Z_L(w)$ with real w) and $a(X) = 0$ whenever $G(\operatorname{supp} X)$ is not connected (just notice that, from definition, $Z_{\operatorname{supp} X}(w) = Z_{L_1}(w) Z_{L_2}(w)$ once $\operatorname{supp} X = L_1 \cup L_2$ with no edges between L_1 and L_2).

In addition, the coefficients $a(X)$ have *alternating signs*:

$$(-1)^{|X|+1} a(X) \geq 0. \tag{8}$$

To prove this claim we verify the validity of an equivalent formulation:

Lemma (alternating signs). *For every finite $L \subset V$, all coefficients of the expansion of $-\log Z_L(-|w|)$ in powers $|w|^X$ are nonnegative.*

Indeed, equivalence with alternating signs property follows by observing that due to (7), one has

$$-\log Z_L(-|w|) = -\sum_{X\in\mathcal{X}(L)} a(X)(-1)^{|X|}|w|^X$$

(and every X has $\operatorname{supp} X \subset L$ for some finite L).

Proof. Proof of the Lemma by induction in $|L|$:

Using a shorthand $Z_L^* = Z_L(-|w|)$, we notice that

$$Z_\emptyset^* = 1 \text{ with } -\log Z_\emptyset^* = 0 \quad \text{ and } \quad Z_{\{v\}}^* = 1 - |w(v)| \text{ with } -\log Z_{\{v\}}^* = \sum_{n=1}^{\infty} \frac{|w(v)|^n}{n}.$$

Using $\mathcal{N}(v)$ to denote the set of vertices $v' \in V$ adjacent in graph G to the vertex v, for w small and $\bar{L} = L \cup \{v\}$, from definition one has $Z_{\bar{L}}^* = Z_L^* - |w(v)| Z_{L\setminus\mathcal{N}(v)}^*$ yielding

$$-\log Z_{\bar{L}}^* = -\log Z_L^* - \log\left(1 - |w(v)| \frac{Z_{L\setminus\mathcal{N}(v)}^*}{Z_L^*}\right)$$

(we consider $|w|$ for which all concerned Taylor expansions for $\log Z_W^*$ with $W \subset \bar{L}$ converge). The first term on the RHS has nonnegative coefficients by induction hypothesis. Taking into account that $-\log(1-z)$ has only nonnegative coefficients and that

$$\frac{Z_{L\setminus\mathcal{N}(v)}^*}{Z_L^*} = \exp\left\{ \sum_{X\in\mathcal{X}(L)\setminus\mathcal{X}(L\setminus\mathcal{N}(v))} |a(X)||w|^X \right\}$$

has also only nonegative coefficients, all the expression on the RHS have necessarily only nonnegative coefficients. □

What is the *diameter of convergence*?

For each finite $L \subset V$, consider the polydiscs $\mathcal{D}_{L,\boldsymbol{R}} = \{w : |w(v)| \le R(v) \text{ for } v \in L\}$ with the set of radii $\boldsymbol{R} = \{R(v); v \in V\}$. The most natural for the inductive proof (leading in the same time to the strongest claim) turns out to be the Dobrushin condition:

There exists a function $r : V \to [0,1)$ such that, for each $v \in V$,

$$R(v) \le r(v) \prod_{v'\in\mathcal{N}(v)} \big(1 - r(v')\big). \tag{$*$}$$

Saying that $X \in \mathcal{X}$ is a cluster if the graph $G(\operatorname{supp} X)$ is connected, we can summarise the cluster expansion claim for an abstract polymer model in the following way:

Theorem (Cluster expansion). *There exists a function $a : \mathcal{X} \to \mathbb{R}$ that is nonvanishing only on* clusters*, so that for any sequence of radii $\boldsymbol{R}$ satisfying the condition $(*)$ with a sequence $\{r(v)\}$, the following holds true:*

(i) *For every finite* $L \subset V$*, and any contour weight* $w \in \mathcal{D}_{L,\boldsymbol{R}}$*, one has* $Z_L(w) \neq 0$ *and*

$$\log Z_L(w) = \sum_{X \in \mathcal{X}(L)} a(X) w^X;$$

(ii) $\sum_{X \in \mathcal{X}:\operatorname{supp} X \ni v} |a(X)||w|^X \leq -\log\bigl(1 - r(v)\bigr)$.

Proof. Again, by induction in $|L|$ we prove (i) and $(\text{ii})_L$ obtained from (ii) by restricting the sum to $X \in \mathcal{X}(L)$:

Assuming $Z_L \neq 0$ and

$$\sum_{X \in \mathcal{X}(L):\operatorname{supp} X \cap \mathcal{N}(v) \neq \emptyset} |a(X)||w|^X \leq -\sum_{v' \in \mathcal{N}(v)} \log\bigl(1 - r(v')\bigr)$$

obtained by iterating $(\text{ii})_L$, we use

$$Z_{\bar{L}} = Z_L \biggl(1 + w(v) \frac{Z_{L \setminus \mathcal{N}(v)}}{Z_L}\biggr)$$

and the bound

$$\left|1 + w(v) \frac{Z_{L \setminus \mathcal{N}(v)}}{Z_L}\right| \geq 1 - |w(v)| \exp\Bigl\{\sum_{X \in \mathcal{X}(L) \setminus \mathcal{X}(L \setminus \mathcal{N}(v))} |a(X)||w|^X\Bigr\} \geq$$

$$\geq 1 - |w(v)| \prod_{v' \in \mathcal{N}(v)} (1 - r(v'))^{-1} \geq 1 - r(v) > 0$$

to conclude that $Z_{\bar{L}} \neq 0$.

To verify $(\text{ii})_{\bar{L}}$, we write

$$\sum_{X \in \mathcal{X}(\bar{L}), \operatorname{supp} X \ni v} |a(X)||w|^X = -\log Z^*_{\bar{L}} + \log Z^*_L = -\log\biggl(1 - |w(v)| \frac{Z^*_{L \setminus \mathcal{N}(v)}}{Z^*_L}\biggr) \leq -\log(1 - r(v)).$$

□

3. Harvesting

3.1. **Ising model at low temperatures.** The low temperature expansion is an instance of an abstract polymer model. Contours γ are its vertices with intersecting pairs connected by an edge:

$$Z_{\Lambda,+}(\beta, 0) = e^{\beta E(\Lambda)} \sum_{\Gamma \text{ in } \Lambda} \underbrace{e^{-2\beta \sum_{\gamma \in \Gamma} |\gamma|}}_{w(\gamma)} = e^{\beta E(\Lambda)} \sum_{I \subset L(\Lambda)} \prod_{\gamma \in I} w(\gamma).$$

Here $L(\Lambda)$ is the set of all contours in Λ.

Checking that (for β large) the weigts $w \in D_R$:

assume that β is large enough so that

$$\sum_{A(\gamma')\ni x} e^{-(2\beta-1)|\gamma'|} \leq 1$$

(for any fixed $x \in \mathbb{Z}^d$ and $A(\gamma') = \{x \in \mathbb{Z}^d : \text{dist}(x, \gamma') \leq 1\}$).
Then choose $r(\gamma) = 1 - \exp\{-e^{-(2\beta-1)|\gamma|}\}$ and verify (instead of $(*)$) the weaker [KP86] condition

$$|w(\gamma)| \leq -(1 - r(\gamma)) \prod_{\gamma' \in \mathcal{N}(\gamma)} (1 - r(\gamma')) \log(1 - r(\gamma))$$

as

$$e^{-2\beta|\gamma|} \leq e^{-(2\beta-1)|\gamma|} \underbrace{\exp\{-e^{-(2\beta-1)|\gamma|} - \sum_{\gamma' \in \mathcal{N}(\gamma)} e^{-(2\beta-1)|\gamma'|}\}}_{\geq e^{-|\gamma|}}$$

(It implies $(*)$ since $-(1-t)\log(1-t) \leq t$.)

Thus the cluster expansion applies:

$$\boxed{\log Z_{\Lambda,+}(\beta, 0) = \beta|E(\Lambda)| + \textstyle\sum_{X \in \mathcal{X}(L(\Lambda))} a(X) w^X}$$

Dependence on Λ only through the set of used multiindeces, *individual terms are* Λ*-independent*!

It implies an explicit expression for the free energy:

$$\boxed{-\beta f(\beta, 0) = \lim \tfrac{\log Z_{\Lambda,+}(\beta,0)}{|\Lambda|} = d\beta + \textstyle\sum_{X \in \mathcal{X}: A(X) \ni x} \tfrac{a(X) w^X}{|A(X)|}}$$

where $A(X) = \cup_{\gamma \in \text{supp} X} A(\gamma)$.

Indeed,

$$\log Z_\Lambda - (-\beta f)|\Lambda| = \beta|E(\Lambda)| - d\beta + \sum_{x \in \Lambda} \Big(\sum_{X \in \mathcal{X}(L(\Lambda)): A(X) \ni x} \frac{a(X) w^X}{|A(X)|} - \sum_{X: A(X) \ni x} \frac{a(X) w^X}{|A(X)|} \Big) \leq$$

$$\leq \beta O(|\partial\Lambda|) + \sum_{X \notin \mathcal{X}(L(\Lambda)): A(X) \ni x} \frac{|a(X)| w^X}{|A(X)|} \leq \beta O(|\partial\Lambda|) + \sum_{y \in \partial\Lambda} e^{-\beta|x-y|} \sum_{X: A(X) \ni y} |a(X)| (\sqrt{w})^X \leq$$

$$\leq \beta O(|\partial\Lambda|) + \sum_{y \in \partial\Lambda} \sum_{x \in \Lambda} e^{-\beta|x-y|} = \beta O(|\partial\Lambda|).$$

Thus, there exists β_0 such that

$$\boxed{f(\beta, 0) \text{ is analytic on } (\beta_0, \infty)}$$

(being, at this interval, an absolutely convergent series of analytic functions in β).

Similarly, at high temperatures: there exists β_1 such that

$$\boxed{f(\beta, h) \text{ is real analytic in } \beta \text{ and } h \text{ for } (\beta, h) : \beta < \beta_1, \beta h < 1.}$$

3.2. **Applications in discrete mathematics.**

3.2.1. *Zeros of the chromatic polynomial.* Sokal [Sok01], Borgs [Bor06]

For a graph $G = (V, E)$ let

$$P_G(q) = \sum_{E' \subset E} q^{C(E')} (-1)^{|E'|}$$

with $C(E')$ denoting the number of components of the graph (V, E').

Theorem. *Let G be of a maximal degree D and $K = \min_a \frac{a+e^a}{\log(1+ae^{-a})}$. Then all zeros of $P_G(q)$ lie inside the disc $\{q \in \mathbb{C}; |q| < DK\}$.*

Idea of proof: $\Phi(G) := \sum_{\substack{E' \subset E \\ E' \text{ connected}}} (-1)^{|E'|}$.

E' yields a partition π. Resum over all $E' \to \pi$:

$$P_G(q) = \sum_{\pi \text{ of } V} \prod_{\gamma \in \pi} \bigl(q \Phi(G(\gamma))\bigr) = q^{|V|} \sum_{\pi \text{ of } V} \prod_{\substack{\gamma \in \pi \\ |\gamma| \geq 2}} \underbrace{\bigl(q^{1-|\gamma|} \Phi(G(\gamma))\bigr)}_{w(\gamma)}.$$

3.2.2. *Connection with Lovász local lemma.* "Bad events" A_v not too strongly dependent (bounded influence outside of a "neighbourhood" of v) $\implies$ there is a positive probability that none of them occurs:

Theorem (Lovász). *$G = (V, E)$, $A_v, v \in V$ family of events, $r(v) \in (0, 1)$ such that $\forall Y \subset V \setminus (N(v) \cup \{v\})$,*

$$P\bigl(A_v \mid \cap_{v' \in Y} \overline{A_{v'}}\bigr) \leq r(v) \prod_{v' \in N(v)} (1 - r(v')).$$

Then

$$P\bigl(\cap_{v \in V} \overline{A_v}\bigr) \geq \prod_{v \in V} (1 - r(v)) > 0.$$

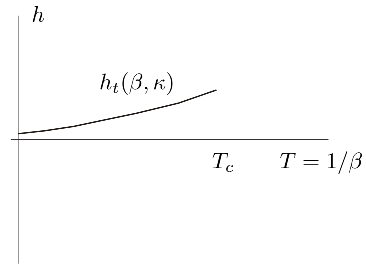
Scott-Sokal [SS05]: $P\bigl(A_v \mid \cap_{v' \in Y} \overline{A_{v'}}\bigr) \leq R(v) \implies P\bigl(\cap_{v \in V}\bigr) \geq Z_G(-R) > 0$ once $R(v) \leq r(v) \prod_{v' \in N(v)} (1 - r(v'))$.

4. Models without symmetry

For example: Ising with

$$H \to H + \kappa \sum \sigma_x \sigma_y \sigma_z$$

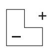
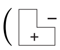
should yield a phase diagram:



Can $h_t(\beta, h)$ be computed?
Can contour representation be used?
The answer is: Yes—with some tricks (Pirogov-Sinai theory [PS75, PS76, Zah84, Kot06]).
Main ideas:
Again,

$$Z_{\Lambda,+}(\beta, h) = e^{\beta|E(\Lambda)|} \sum_{\Gamma \text{in } \Lambda} e^{-\beta e_+|\Lambda_+(\Gamma)| - \beta e_-|\Lambda_-(\Gamma)|} \prod_{\gamma\in\Gamma} w(\gamma).$$

However, contours cannot be erased without changing the remaining configuration:

- $\Lambda_\pm(\Gamma)$ changes,
- $w($$) \neq w($$)$.

Actually, we have here *labeled contours* with *"hard-core long range interaction"*.

First trick: restoring independence. The cost of erasing γ including flipping of the interior:

$$w_+(\gamma) = w(\gamma)\frac{Z_{\text{Int}\gamma,-}}{Z_{\text{Int}\gamma,+}}, \qquad w_-(\gamma) = w(\gamma)\frac{Z_{\text{Int}\gamma,+}}{Z_{\text{Int}\gamma,-}}.$$

We get

$$Z_{\Lambda,+} = e^{-\beta e_+|\Lambda|} \sum_{\Gamma \text{ in } \Lambda} \prod_{\gamma\in\Gamma} w_+(\gamma)$$

by induction in $|\Lambda|$:

$$Z_{\Lambda,+} = \sum_{\theta \text{ exterior contours}} e^{-\beta e_+|\text{Ext}\theta|} \prod_{\gamma\in\theta} \underbrace{w(\gamma)\frac{Z_{\text{Int}\gamma,-}}{Z_{\text{Int}\gamma,+}}}_{w_+(\gamma)} Z_{\text{Int}\gamma,+},$$

with $Z_{\text{Int}\gamma,+} = e^{-\beta e_+|\text{Int}\gamma|} \sum$ by induction step.

The contour partition function $Z_{L(\Lambda)}(w_+)$ yields the same probability for external contours as original physical system.

If $w_+(\gamma)| \leq e^{-\tau|\gamma|}$ with large $\tau \implies$ typical configuration is a sea of pluses with small islands.

For any (h, β) with β large, either w_+ or w_- (or both) should be supressed. But which one?

Second trick: metastable states. Define

$$\overline{w_\pm}(\gamma) := \begin{cases} w_\pm(\gamma) \text{ if } w_\pm(\gamma) \le e^{-\tau|\gamma|} \\ e^{-\tau|\gamma|} \text{ otherwise} \end{cases}$$

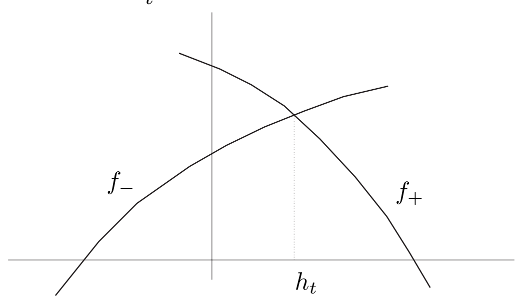
and

$$\overline{Z}_{\Lambda,\pm} := e^{-\beta e_\pm |\Lambda|} \underbrace{Z_{L(\Lambda)}(\overline{w_\pm})}_{\text{cluster exp.}\to g(\overline{w_\pm})}$$

with $-\beta \log \overline{Z}_{\Lambda,\pm} \sim |\Lambda| f_\pm$, where $f_\pm := e_\pm + g(\overline{w_\pm})$.

Notice: f_+ and f_- are inductively (through $\overline{w_\pm}$) unambiguously defined.

Once we have them, we can introduce h_t:



The final step is to prove (again by a careful induction):

$h \le h_t \to f_- = \min(f_-, f_+) \implies \overline{w_-} = w_-$ $(\&\overline{w_+}(\gamma) = w_+(\gamma)$ for $\gamma : \beta(f_+ - f_-)\mathrm{diam}\gamma \le 1)$

and

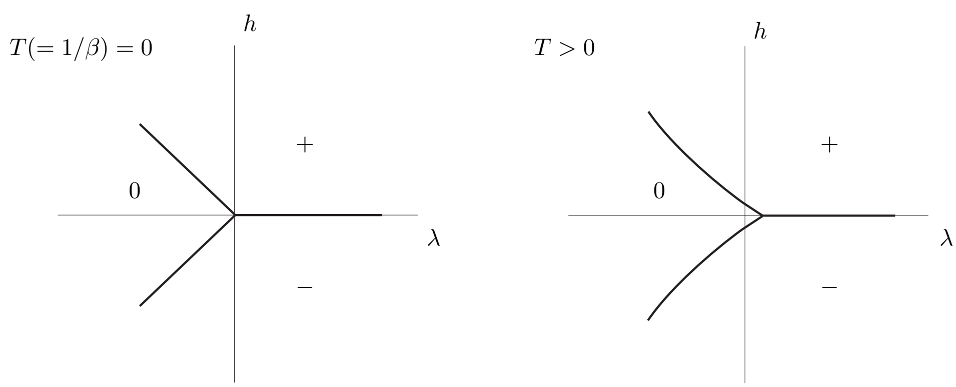
$h \ge h_t \to f_+ = \min(f_-, f_+) \implies \overline{w_+} = w_+$ $(\&\overline{w_-}(\gamma) = w_-(\gamma)$ for $\gamma : \beta(f_- - f_+)\mathrm{diam}\gamma \le 1)$.

Standard example: Blume-Capel model.

Spin takes three values, $\sigma_x \in \{-1, 0, 1\}$, with Hamiltonian

$$\sum_{\langle x,y\rangle} (\sigma_x - \sigma_y)^2 - \lambda \sum \sigma_x^2 - h \sum \sigma_x.$$

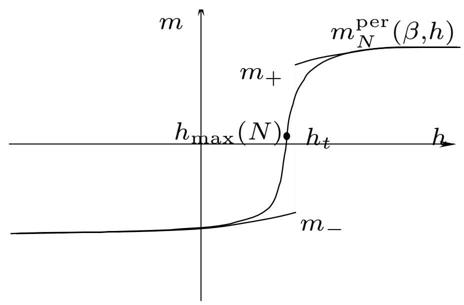
The phase diagram features three competing phases: $+$, $-$, and 0:



For the origin $h = \lambda = 0$, the phase 0 is stable ($f_0 > f_+, f_-$):
indeed, one has $e_+ = e_- = e_0 = 0$, and $g(\overline{w_\pm}) \sim -e^{-4\beta} > g(\overline{w_0}) \sim -2e^{-4\beta}$ (lowest excitations: one 0 in the sea of + (or −), while, favourably, either one + or one − (*two possibilities*) in the sea of 0).

5. Second harvest

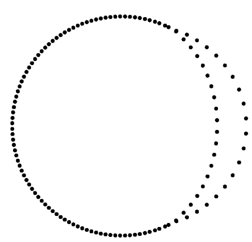
Finite volume asymptotics:
Using Pirogov-Sinai theory, one has a good control over the finite volume behaviour.
For example, say, for the Ising model with an asymmetry, we get an asymptotics of the magnetization $m_N^{\mathrm{per}}(\beta, h)$ in volume N^d with periodic boundary conditions [BK90]:



In particular,

$$h_{\max}(N) = h_t + \frac{3\chi}{2\beta^2 m^3} N^{-2d} + O(N^{-3d}).$$

Zeros of partition function: Blume-Capel in $z = e^{-\beta h}$ for the partition function Z_N^{per} with periodic boundary conditions:



One can obtain results about asymptotic loci of zeros by analyzing

$$Z^{\mathrm{per}} \sim e^{-\beta f_+ N^d} + e^{-\beta f_- N^d} + e^{-\beta f_0 N^d}$$

obtained with help of a complex extension of Pirogov-Sinai and cluster expansions [BBCKK04, BBCK04].

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