Cluster expansions for hard-core systems. I. Introduction

Roberto Fernández
CNRS - Université de Rouen

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The setup

Goal: To study systems of objects constrained only by a "non-overlapping" condition

Countable family $\mathcal{P}$ of objects: polymers, animals, ..., characterized by

- An *incompatibility* constraint:

$$\begin{matrix} \gamma \nsim \gamma' \\ \gamma \sim \gamma' \end{matrix} \quad \text{if } \gamma, \gamma' \in \mathcal{P} \qquad \begin{matrix} \text{incompatible} \\ \text{compatible} \end{matrix}$$

  For simplicity: each polymer incompatible with itself ($\gamma \nsim \gamma, \forall \gamma \in \mathcal{P}$)

- A family of *activities* $\boldsymbol{z} = \{z_\gamma\}_{\gamma \in \mathcal{P}} \in \mathbb{C}^{\mathcal{P}}$.

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The basic ("finite-volume") measures

Defined, for each *finite* family $\Lambda \subset \mathcal{P}$, by weights

$$\mathrm{W}_\Lambda\big(\{\gamma_1, \gamma_2, \ldots, \gamma_n\}\big) \;=\; \frac{1}{\Xi_\Lambda(\boldsymbol{z})}\, z_{\gamma_1} z_{\gamma_2} \cdots z_{\gamma_n} \prod_{j<k} \mathbb{1}_{\{\gamma_j \sim \gamma_k\}}$$

for $n \geq 1$ $\gamma_1, \gamma_2, \ldots, \gamma_n \in \Lambda$, and $\mathrm{W}_\Lambda(\emptyset) = 1/\Xi_\Lambda$, where

$$\Xi_\Lambda(\boldsymbol{z}) = 1 + \sum_{n \geq 1} \frac{1}{n!} \sum_{(\gamma_1, \ldots, \gamma_n) \in \Lambda^n} z_{\gamma_1} z_{\gamma_2} \cdots z_{\gamma_n} \prod_{j<k} \mathbb{1}_{\{\gamma_j \sim \gamma_k\}}$$

The questions:

- Existence of the limit $\Lambda \to \mathcal{P}$ ("thermodynamic limit")
- Properties of the resulting measure (mixing properties, dependency on parameters,...)

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Immediate:

- *Physics:* Grand-canonical ensemble of polymer gas with activities z_γ and hard-core interaction
- *Statistics:* Invariant measure of point processes with not-overlapping grains and birth rates z_γ

Less immediate:

- Statistical mechanical models at high and low temperatures are mapped into such systems
- More generally: most perturbative arguments in physics involve maps of this type (choice of the "right" variables)
- Zeros of the partition functions Ξ_Λ relate to phase transitions (sphere packing, chromatic polynomials,...)

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Graph-theoretical framework

Equivalently, consider the *interaction graph* $\mathcal{G} = (\mathcal{P}, \mathcal{E})$

Unoriented graph with:

- Vertices = polymers
- Edges = incompatible pairs

$$\gamma \nsim \gamma' \quad \text{iff} \quad \{\gamma, \gamma'\} \in \mathcal{E} \quad \text{or} \quad \gamma \leftrightarrow \gamma' \tag{1}$$

(contrast!)

- $\mathcal{E}$ is arbitrary; vertices can be of infinite degree (polymers incompatible with infinitely many other polymers)
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Example: Single-call loss networks

Definition

- $\mathcal{P}$ = finite subsets of $\mathbb{Z}^d$ —the *calls*
- A call γ is attempted with Poissonian rates z_γ
- Call succeeds if it does not intercept existing calls
- Once established, calls have an exp(1) life span

Remarks

- Basic measures are invariant for the finite-region process ($\gamma \propto \gamma' \Longleftrightarrow \gamma \cap \gamma' \neq \emptyset$)
- Thermodynamic limit: infinite-volume process
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Statistical mechanical lattice models

Their ingredients are:

- *Lattice* $\mathbb{L}$ countable set of sites (e.g. $\mathbb{Z}^d$)
- *Single-site space* $(E, \mathcal{F}, \mu_E)$ with natural measure structure (e.g. counting measure if E countable, Borel if $E \subset \mathbb{R}^d$)
- *Configuration space* $\Omega = E^{\mathbb{L}}$, with product measure
- *Interaction* $\Phi = \{\phi_B : B \subset\subset \mathbb{L}\}$ where $\phi_B = \phi_B(\omega_B)$. [*Bond:* B such that $\phi_B \neq 0$]
- *Hamiltonians:* For $\Lambda \subset\subset \mathbb{L}$, and boundary condition σ

$$H_\Lambda(\omega \mid \sigma) = \sum_{B \subset \Lambda} \phi_B(\omega_\Lambda \sigma)$$

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Statistical mechanical measures

Their finite-volume versions are defined by weights

$$W_\Lambda(\omega \mid \sigma) \;=\; \frac{\exp\{-\beta H_\Lambda(\omega \mid \sigma)\}}{Z^\sigma_\Lambda}$$

with

$$Z^\sigma_\Lambda \;=\; \int \exp\{-\beta H_\Lambda(\omega \mid \sigma)\} \bigotimes_{x\in\Lambda} \mu_E(d\omega_x)$$

($\beta =$ inverse temperature)

Ising model at low temperatures

$\mathbb{L} = \mathbb{Z}^d$, $E = \{-1, 1\}$, $\mathcal{F}$ =discrete, μ_E =counting

$$\phi_B(\omega) \;=\; \begin{cases} -J\,\omega_x\omega_y & \text{if } B = \{x, y\} \text{ n.n.} \\ 0 & \text{otherwise} \end{cases}$$

Call a bond $B = \{x, y\}$ *frustrated* if $\omega_x\omega_y = -1$

$$H_\Lambda(\omega \mid +) \;=\; 2J\,F_\Lambda(\omega) - JN_\Lambda\;;$$

$$\begin{aligned} F_\Lambda(\omega) &= \#\{B \text{ frustrated} : B \cap \Lambda \neq \emptyset\} \\ N_\Lambda &= \#\{B : B \cap \Lambda \neq \emptyset\} \end{aligned}$$

As N_Λ is independent of ω

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Contour representation

- Place a plaquette (segment) orthogonally at the midpoint of each frustrated bond
- These plaquettes form a family of disjoint closed connected surfaces (curves)
- Each such closed surface is a *contour*
- Contours are disjoint: $\gamma \sim \gamma' \iff \gamma \cap \gamma' = \emptyset$
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Contour polymer model

$$\exp\Big\{-2\beta J\, F_\Lambda(\omega)\Big\} \;=\; \exp\Big\{-\sum_{\gamma\in\Gamma(\omega)} 2\beta J\ |\gamma|\Big\}$$
$$= \prod_{\gamma\in\Gamma(\omega)} z_\gamma$$

with $z_\gamma = \exp\{-2\beta J\ |\gamma|\}$. Hence

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Geometrical polymer models

Polymers of previous two examples are defined by parts of a set

These are the original polymer models of Gruber and Kunz

Formally, geometrical polymer models are defined by:

- A set $\mathbb{V}$
- A family $\mathcal{P}$ of finite subsets of $\mathbb{V}$
- Activity values $(z_\gamma)_{\gamma \in \mathbb{V}}$
- The relation $\gamma \sim \gamma' \iff \gamma \cap \gamma' = \emptyset$

More generally, $\mathbb{V}$ can be the vertex set of a graph and

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Ratios of partition functions

Physicists are obsessed with (logs of) partition functions

Three reasons why they are right:

- Probabilities of cylindrical events are ratios of partition functions
- So are characteristic and moment-generating functions
- (Complex) zeros of partition functions related to phase transitions, coloring problems, etc

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Cylindrical polymer events

Let

- Prob_Λ the basic measure in Λ
- $\gamma_1, \ldots, \gamma_k$ mutually compatible polymers in Λ

Then

$$\text{Prob}_\Lambda\big(\{\gamma_1, \ldots, \gamma_k \text{ are present}\}\big) \;=\; z_{\gamma_1} \cdots z_{\gamma_k} \, \frac{\Xi_{\Lambda \setminus \{\gamma_1, \ldots, \gamma_k\}^*}}{\Xi_\Lambda}$$

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Characteristic/moment-generating functions

Let $\alpha : \mathcal{P} \to \mathbb{R}$ and

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for $\{\gamma_1, \ldots, \gamma_n\} \subset \Lambda$. Hence $E_\Lambda\big(\mathrm{e}^{\xi\, S_\Lambda}\big)$ equals

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Zeros and phase transitions

For (translation-invariant) stat-mech models

$$f(\beta, \boldsymbol{h}) \;=\; \lim_{\Lambda \to \mathbb{L}} \frac{1}{|\Lambda|} \log Z^{\sigma}_{\Lambda}$$

exists and is independent of the boundary condition σ

Key information: smoothness as function of β and $\boldsymbol{h}$

"Functions should be analytic unless there is a good reason"

Loss of analyticity = phase transition (of some sort)

Sufficient conditions for analyticity of f:

- Zeros of Z_Λ Λ-uniformly away from $(\beta, \boldsymbol{h})$
- Λ-independent radius of analyticity of $\frac{1}{|\Lambda|} \log Z_\Lambda$

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- Zeros of Z_Λ Λ-uniformly away from $(\beta, \boldsymbol{h})$
- Λ-independent radius of analyticity of $\frac{1}{|\Lambda|} \log Z_\Lambda$

Alternative lines of attack

Physicist:

Control Ξ through expansion techniques $\longrightarrow$ cluster expansions

- Genesis/reincarnations: Mayer, virial, high-temperature, low-density, . . . expansions
- Not everybody's cup of tea
- Involves algebraic and graph theoretical considerations
- Less natural for purely probabilistic studies (analyticity?)

Probabilists:

Models with exclusions = invariant measures of point processes

- Weaker results (no analyticity!) but wider applicability
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Cluster expansions

The idea is to write the polynomials in $(z_\gamma)_{\gamma\in\mathcal{P}}$

$$\Xi_\Lambda(\boldsymbol{z}) = 1 + \sum_{n\geq 1} \frac{1}{n!} \sum_{(\gamma_1,\dots,\gamma_n)\in\Lambda^n} z_{\gamma_1} z_{\gamma_2} \dots z_{\gamma_n} \prod_{j<k} \mathbb{1}_{\{\gamma_j\sim\gamma_k\}}$$

as *formal* exponentials of another *formal* series

$$\Xi_\Lambda(\boldsymbol{z}) \stackrel{\text{F}}{=} \exp\Big\{ \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{(\gamma_1,\dots,\gamma_n)\subset\Lambda^n} \phi^T(\gamma_1,\dots,\gamma_n)\, z_{\gamma_1}\dots z_{\gamma_n} \Big\}$$

The series between curly brackets is the *cluster expansion*

- $\phi^T(\gamma_1,\dots,\gamma_n)$: *Ursell* or *truncated* functions (symmetric)
- *Clusters*: Families $\{\gamma_1,\dots,\gamma_n\}$ s.t. $\phi^T(\gamma_1,\dots,\gamma_n)\neq 0$
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Ratios and derivatives

Telescoping, ratios of partitions = product of one-contour ratios

Substracting cluster expansions:

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Slightly more convenient series:

$$\frac{\partial}{\partial z_{\gamma_0}}\log\Xi_\Lambda \stackrel{\mathrm{F}}{=} 1+\sum_{n=1}^{\infty}\frac{1}{n!}\sum_{(\gamma_1,\dots,\gamma_n)\subset\Lambda^n} \phi^T(\gamma_0,\gamma_1,\dots,\gamma_n)\, z_{\gamma_1}\cdots z_{\gamma_n}$$

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Two strategies to deal with this series: *classical* and *inductive*

Classical cluster-expansion strategy

Find convergence conditions for the series

$$\Pi_{\gamma_0}(\boldsymbol{\rho}) \;:=\; 1+\sum_{n=1}^{\infty}\frac{1}{n!}\sum_{(\gamma_1,\ldots,\gamma_n)\in\mathcal{P}^n}\left|\phi^T(\gamma_0,\gamma_1,\ldots,\gamma_n)\right|\,\rho_{\gamma_1}\cdots\rho_{\gamma_n}$$

for $\rho_\gamma > 0$. Then,

Cluster expansions converge *absolutely* for $|z_\gamma| \leq \rho_\gamma$ *uniformly in* Λ (complex valued allowed!)

This determines a region of analyticity $\mathcal{R}$ *common for all* Λ

Within this region

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Consequences

- Zeros of all Ξ_Λ outside $\mathcal{R}$ (no phase transitions!)
- Within $\mathcal{R}$
  - Explicit series expressions for free energy and correlations
  - Explicit δ-mixing:

$$\left| \frac{\mathrm{Prob}(\{\gamma_0\,,\,\gamma_x\})}{\mathrm{Prob}(\{\gamma_0\})\,\mathrm{Prob}(\{\gamma_x\})} - 1 \right| \;=\; \left| \mathrm{e}^{F[d(\gamma_0,\gamma_x)]} - 1 \right|$$

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Free energy expansions

For geometrical translation-invariant polymers,

$$\begin{aligned} f &= \lim_{\Lambda} \frac{1}{|\Lambda|} \log \Xi_\Lambda \\ &= \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{(\gamma_1,\ldots,\gamma_n)\,:\,0\in\cup\gamma_i} \phi_n^T(\gamma_1,\ldots,\gamma_n)\, z_{\gamma_1}\ldots z_{\gamma_n} \end{aligned}$$

As

$$\phi^T(\gamma) = 1 \quad , \quad \phi^T(\gamma,\gamma') = \begin{cases} -1 & \text{if } \gamma \nsim \gamma' \\ 0 & \text{otherwise} \end{cases}$$

$$f = \sum_{\gamma \ni 0} z_\gamma - \frac{1}{2} \sum_{\gamma \nsim \gamma'} z_\gamma\, z_{\gamma'} + O(|\boldsymbol{z}|^3)$$

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Inductive strategy (Kotecký-Preiss, Dobrushin)

Find conditions on $\mathbf{z}$ defining a region $\mathcal{R}$ such that

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for all Λ, $\gamma_0 \notin \Lambda$

- Expansion neither needed nor obtained (*no-cluster-expansion* method)
- A posteriori: expansion converges in $\mathcal{R} \longrightarrow$ above concl.

Questions raised

- Why the alternative approach lead to better results?
- Can it be interpreted in terms of the classical approach?

Answer: Classical theory revisited

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Associated polymer models

A model has an associated polymer model if partition ratios are the same

Equivalently,

$$Z_\Lambda^{\text{model}}(\text{param.}) \;=\; \text{const}_\Lambda \, \Xi_\Lambda^{\text{polymer}}(\boldsymbol{z})$$

($\text{const}_\Lambda \sim a^{|\Lambda|}$). Will see two examples

Useful observation

If S finite set and $(\varphi_a)_{a\in S}$, $(\psi_a)_{a\in S}$ complex-valued:

$$\prod_{a\in S}[\psi_a+\varphi_a] = \sum_{A\subset S}\prod_{a\in A}\varphi_a \prod_{a\in S\setminus A}\psi_a$$

$[\prod_\emptyset \equiv 1]$

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Potts model

$\mathbb{L}$ any (eg. $\mathbb{Z}^d$), $E = \{1, \ldots, q\}$, $\mathcal{F}$ =discrete, μ_E =counting

$$\phi_B(\omega) \;=\; \begin{cases} -J_{x\,y}\left(\delta_{\omega_x \omega_y} - 1\right) & \text{if } B = \{x, y\} \text{ n.n.} \\ 0 & \text{otherwise} \end{cases}$$

- $\phi_{\{x,y\}} = J$ if $\omega_x \neq \omega_y$, 0 otherwise
- If $q = 2$, Potts=Ising

$$Z_\Lambda^{\text{Potts}}(\beta, q) \;=\; \sum_{\omega_\Lambda} \prod_{\{x,y\} \subset \Lambda} \mathrm{e}^{\beta J_{x\,y}(\delta_{\omega_x \omega_y} - 1)}$$

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The FK trick

Crucial observation:

$$\mathrm{e}^{\beta J_{x\,y}(\delta_{\omega_x\omega_y}-1)} = \delta_{\omega_x\omega_y} + \mathrm{e}^{-\beta J_{x\,y}}(1-\delta_{\omega_x\omega_y})$$

$$= (1-p_{x\,y}) + p_{x\,y}\,\delta_{\omega_x\omega_y}$$

with $p_{x\,y} = 1 - \mathrm{e}^{-\beta J_{x\,y}}$. Hence

$$Z_\Lambda^{\mathrm{Potts}}(\beta,q) = \sum_{\omega_\Lambda} \prod_{\{x,y\}\subset\Lambda} \Big[(1-p_{x\,y}) + p_{x\,y}\,\delta_{\omega_x\omega_y}\Big]$$

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($\mathcal{B}$ = bonds)

The FK trick

Crucial observation:

$$\begin{aligned} \mathrm{e}^{\beta J_{x\,y}(\delta_{\omega_x\omega_y}-1)} &= \delta_{\omega_x\omega_y} + \mathrm{e}^{-\beta J_{x\,y}}(1-\delta_{\omega_x\omega_y}) \\ &= (1-p_{x\,y}) + p_{x\,y}\,\delta_{\omega_x\omega_y} \end{aligned}$$

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The FK expansion

As

$$\sum_{\omega_\Lambda} \prod_{\{x,y\}\in \boldsymbol{B}} \delta_{\omega_x \omega_y} \;=\; q^{C(\boldsymbol{B})}$$

with $C(\boldsymbol{B}) = \#$ connected components of $\boldsymbol{B}$,

$$Z_\Lambda^{\text{Potts}}(\beta, q) \;=\; \sum_{\boldsymbol{B}\subset\mathcal{B}} q^{C(\boldsymbol{B})} \prod_{\{x,y\}\in \boldsymbol{B}} p_{x\,y} \prod_{\{x,y\}\notin \boldsymbol{B}} (1 - p_{x\,y})$$

- $q = 1$: regular (independent) bond percolation in $\mathbb{Z}^d$
- $q > 1$: dependent percolation due to $q^{C(\boldsymbol{B})}$

FK model

$$Z_\Lambda^{\text{Potts}}(\beta, q) = \Big[\prod_{\{x,y\}\in\mathcal{B}} (1 - p_{x\,y})\Big] \sum_{\boldsymbol{B}\subset\mathcal{B}} q^{C(\boldsymbol{B})} \prod_{\{x,y\}\in\boldsymbol{B}} \frac{p_{x\,y}}{1 - p_{x\,y}}$$

$$= \Big[\prod_{\{x,y\}\in\mathcal{B}} (1 - p_{x\,y})\Big] Z_\Lambda^{\text{FK}}(q, \boldsymbol{v})$$

with

$$Z_\Lambda^{\text{FK}}(q, \boldsymbol{v}) = \sum_{\boldsymbol{B}\subset\mathcal{B}} q^{C(\boldsymbol{B})} \prod_{\{x,y\}\in\boldsymbol{B}} v_{x\,y}$$

and

$$v_{x\,y} = \frac{p_{x\,y}}{1 - p_{x\,y}} = \mathrm{e}^{\beta\, J_{x\,y}} - 1$$

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FK polymer model

(Also called *random-cluster model*)

Reorder the sum:

- Each $\boldsymbol{B}$ defines a graph $G = (V_{\boldsymbol{B}}, \boldsymbol{B})$
- Let $G_i = (V_i, \boldsymbol{B}_i)$, $i = 1, \ldots, k$ connected components
  - The vertex sets are disjoints: $V_i \cap V_j = \emptyset$ if $i \neq j$
  - The sets of bonds $\boldsymbol{B}_i$ are such that each G_i is connected

Furthermore

$$\begin{aligned} C(\boldsymbol{B}) &= k + \#\text{ isolated points} \\ &= k + |\Lambda| - \sum |V_i| \\ &= |\Lambda| - \sum (|V_i| - 1) \end{aligned}$$

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High-q expansion

Then

$$\frac{Z_\Lambda^{\mathrm{FK}}(q,\boldsymbol{v})}{q^{|\Lambda|}} = \sum_{k\geq 0}\frac{1}{k!}\sum_{\substack{(V_1,\dots,V_k)\in\Lambda^k\\ \text{disjoints}}}\prod_{i=1}^{k}\Bigg[q^{-(|V_i|-1)}\sum_{\substack{\boldsymbol{B}_i\subset\mathcal{B}_{V_i}\\ (V_i,\boldsymbol{B}_i)\,\text{conn.}}}\prod_{\{x,y\}\in\boldsymbol{B}_i} v_{x\,y}\Bigg]$$

$$= \Xi_\Lambda^{\mathrm{FK}}(\boldsymbol{z})$$

FK geometrical polymer system: $\mathcal{P} = \{V \subset\subset \mathbb{L}\}$,

$$z_V = q^{-(|V|-1)}\sum_{\substack{B\subset\mathcal{B}_V\\ (V,B)\,\text{connected}}}\prod_{\{x,y\}\in B} v_{x\,y}$$

decreases as $q\to\infty$ (or as $\beta\to 0$)

Corresponding cluster expansion = *high-q (high-T) expansion*

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Chromatic polynomials

Given a graph $G = \big(V(G), E(G)\big)$:

$$P_G(q) \;=\; \#\text{ ways of properly coloring } G \text{ with } q \text{ colors}$$

"properly" = adjacents vertices have different colors

If $\omega : V(G) \to \{1, \ldots, q\}$ denote colorings

$$P_G(q) \;=\; \sum_{\omega} \prod_{\{x,y\} \in E(G)} \big[1 - \delta_{\omega_x\, \omega_y}\big]$$

Introduced by Birkhoff (1912) to determine

$$\chi_G \;=\; \min\big\{q : P_G(q) > 0\big\}$$

chromatic number = minimal q for a proper coloring

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Tutte polynomial

Slight generalization: $(-1) \to v_{x\,y}$

$$P_G(q, \boldsymbol{v}) \;=\; \sum_{\omega} \prod_{\{x,y\} \in E(G)} \Big[1 + v_{x\,y}\, \delta_{\omega_x\, \omega_y} \Big]$$

- Dichromatic polynomial
- Dichromate
- Whitney rank function
- Tutte polynomial

For us

$$P_G(q, \boldsymbol{v}) \;=\; Z^{\mathrm{FK}}_{\Lambda}(q, \boldsymbol{v}) \;=\; q^{|\Lambda|}\, \Xi^{\mathrm{FK}}_{\Lambda}(\boldsymbol{z})$$

This identity proves that $P_G(q, \boldsymbol{v})$ is a polynomial in q

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Chromatic numbers and cluster expansions

If $J_{x\,y} < 0$ (antiferromagnetic Potts model)

$$v_{x\,y} = \mathrm{e}^{\beta J_{x\,y}} - 1 \xrightarrow[\beta\to\infty]{} -1$$

Hence

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Region free the zeros of $P_G(q) \to$ bound on χ_G

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