

**Pressure and phase transition in
Potts models in Statistical Mechanics**

Shmuel Friedland
University of Illinois at Chicago

**Seminar in Hebrew University,
December 26, 2006**

Last version December 14, 2006

1 Outline of the talk

- Motivation: Ising model
- Subshifts of Finite Type
- Pressure P_Γ
- Density points and density entropy
- Convex functions
- P_Γ^* and color density entropy
- First order phase transition
- The maximum principle
- d -Dimensional Monomer-Dimers
- Friendly colorings
- Computation of pressure

2 Motivation: Ising model - 1925

On lattice \mathbb{Z}^d two kinds of particles: spin up **1** and spin down **2**. Each neighboring particles located on $(\mathbf{i}, \mathbf{i} + \mathbf{e}_j)$ interact with energy $-J$ if both locations are occupied by the same particles, and with energy J if the two sites are occupied by two different particles. In addition each particle has a magnetization due to the external magnetic field. The energy of the particle of type **1** is H while the energy of the particle of type **2** is $-H$. The energy of $E(\phi)$ of a given finite configuration of particles in \mathbb{Z}^d is the sum of the energies of the above type.

Ferromagnetism $J > 0$: all spins are up or down.

Antiferromagnetism $J < 0$ half spins up and down

(Lowest free energy)

Phase transition:

from one state to another as the temperature varies

Energy: $\frac{k}{T} E(\phi)$

3 Subshifts of Finite Type-SOFT

$$\langle n \rangle := \{1, 2, 3, \dots, n\}$$

ALPHABET ON n LETTERS - COLORS.



Coloring of \mathbb{Z}^d in n coloring =

Full \mathbb{Z}^d shift on n symbols

Example of SOFT: (0 – 1) LIMITED CHANNEL

HARD CORE LATTICE or NEAR NEIGHBOR EXCLUSION

$$n = 2, \langle 2 \rangle = \{1, 2\} = \{1, 0\} (2 \equiv 0).$$

NO TWO 1's ARE NEIGHBORS.

4 One dimensional SOFT

$\Gamma \subseteq \langle n \rangle \times \langle n \rangle$ directed graph on n vertices

$C_\Gamma(\langle m \rangle)$ -all Γ allowable configurations of length m :

$$\{a = a_1 \dots a_m = (a_i)_1^m : \langle m \rangle \rightarrow \langle n \rangle \\ (a_i, a_{i+1}) \in \Gamma\}$$

$C_\Gamma(\mathbb{Z})$ -all Γ allowable configurations (tilings) on \mathbb{Z} :

$$\{a = (a_i)_{i \in \mathbb{Z}} : \mathbb{Z} \rightarrow \langle n \rangle, (a_i, a_{i+1}) \in \Gamma\}$$

Hard core model:

$$n = 2, \Gamma = \{\bullet\bullet, \bullet\bullet, \bullet\bullet\}$$



5 MD SOFT=Potts Models

Dimension $d \geq 2$. For $\mathbf{m} \in \mathbb{N}^d$

$$\langle \mathbf{m} \rangle := \langle m_1 \rangle \times \dots \times \langle m_d \rangle$$

$$\text{vol}(\mathbf{m}) := |m_1| \times \dots \times |m_d|$$

$$\Gamma := (\Gamma_1, \dots, \Gamma_d), \Gamma_i \subset \langle n \rangle \times \langle n \rangle$$

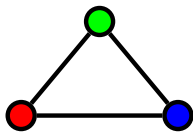
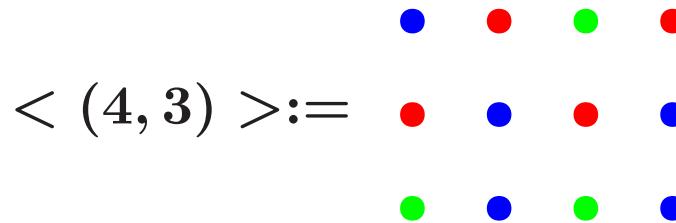
$C_\Gamma(\langle \mathbf{m} \rangle)$ -all Γ allowable configurations of \mathbf{m} :

$$a = (a_i)_{i \in \langle \mathbf{m} \rangle} : \langle \mathbf{m} \rangle \rightarrow \langle n \rangle$$

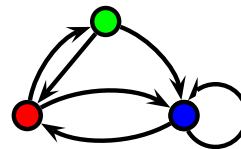
$$\text{s.t. } (a_i, a_{i+e_j}) \in \Gamma_j \text{ if } i, i+e_j \in \langle \mathbf{m} \rangle$$

$$e_j = (\delta_{1j}, \dots, \delta_{dj}), j = 1, \dots, d.$$

Example:



Γ_1



Γ_2

For $\phi \in C_\Gamma(\langle \mathbf{m} \rangle)$ - $\mathbf{c}(\phi) := (c_1(\phi), \dots, c_n(\phi))$

denotes coloring distribution of configuration ϕ

$c_i(\phi)$ -the number of times the particle i appears in ϕ

$\frac{1}{\text{vol}(\mathbf{m})} \mathbf{c}(\phi) \in \Pi_n$ - coloring frequency of ϕ

$\Pi_n(\text{vol}(\mathbf{m}))$ all $\mathbf{c} \in \mathbb{Z}_+^n$ s.t. $\frac{1}{\text{vol}(\mathbf{m})} \mathbf{c} \in \Pi_n$

$C_\Gamma(\langle \mathbf{m} \rangle, \mathbf{c})$ denotes all $\phi \in C_\Gamma(\langle \mathbf{m} \rangle)$ with $\mathbf{c}(\phi) = \mathbf{c}$.

$C_{\Gamma, \text{per}}(\langle \mathbf{m} \rangle) \subseteq C_\Gamma(\langle \mathbf{m} \rangle)$ - \mathbf{m} -periodic configurations

$C_\Gamma(\mathbb{Z}^d)$ -are- Γ allowable configurations of \mathbb{Z}^d

Assumption: $C_\Gamma(\mathbb{Z}^d) \neq \emptyset$

$u_i \in \mathbb{R}$ energy of particle $i \in \langle n \rangle$

$\mathbf{u} := (u_1, \dots, u_n) \in \mathbb{R}^n$ energy vector

$E(\phi) = \mathbf{c}(\phi) \cdot \mathbf{u}$ Energy of configuration ϕ

Near neighbor interaction model, can be fit to the above noninteraction model by considering the coloring of the cube $\langle (\mathbf{3}, \dots, \mathbf{3}) \rangle$ as one particle

Similarly short range interaction model

6 Pressure

Grand partition function

$$Z_{\Gamma}(\mathbf{m}, \mathbf{u}) := \sum_{\phi \in C_{\Gamma}(\langle \mathbf{m} \rangle)} e^{c(\phi) \cdot \mathbf{u}}$$

$\log Z_{\Gamma}(\mathbf{m}, \mathbf{u})$ subadditive in each component of \mathbf{m} and convex in \mathbf{u}

$\frac{1}{\text{vol}(\mathbf{m})} \log Z_{\Gamma}(\mathbf{m}, \mathbf{u})$ - average energy or pressure

$$P_{\Gamma}(\mathbf{u}) := \lim_{\mathbf{m} \rightarrow \infty} \frac{1}{\text{vol}(\mathbf{m})} \log Z_{\Gamma}(\mathbf{m}, \mathbf{u})$$

Pressure of Γ -SOFT, (Pressure of the Potts model)

$h_{\Gamma} := P_{\Gamma}(\mathbf{0})$ - ENTROPY of Γ -SOFT

$P_{\Gamma}(\mathbf{u})$ is a convex Lipschitz function on \mathbb{R}^n

$$|P_{\Gamma}(\mathbf{u}) - P_{\Gamma}(\mathbf{v})| \leq \|\mathbf{u} - \mathbf{v}\|_{\infty} := \max |u_i - v_i|$$

$$P_{\Gamma}(\mathbf{u} + t\mathbf{1}) = P_{\Gamma}(\mathbf{u}) + t$$

P_{Γ} has the following properties:

Has subdifferential $\partial P_{\Gamma}(\mathbf{u})$ for each \mathbf{u}

$$\partial P_{\Gamma}(\mathbf{u}) \subseteq \Pi_n \text{ for each } \mathbf{u}$$

Has differentiable $\nabla P_{\Gamma}(\mathbf{u})$ a.e.

7 Density points and density entropy

$p \in \Pi_n$ density point of $C_\Gamma(\mathbb{Z}^d)$ when there exist sequences of boxes $\langle m_q \rangle \subseteq \mathbb{N}^d$ and color distribution vectors $c_q \in \Pi_n(\text{vol}(m_q))$

$m_q \rightarrow \infty$, $C_\Gamma(\langle m_q \rangle, c_q) \neq \emptyset \quad \forall q \in \mathbb{N}$, and $\lim_{q \rightarrow \infty} \frac{c_q}{\text{vol}(m_q)} = p$

Π_Γ the set of all density points of $C_\Gamma(\mathbb{Z}^d)$

Π_Γ is a closed set

For $p \in \Pi_\Gamma$ the color density entropy

$$h_\Gamma(p) := \sup_{m_q, c_q} \limsup_{q \rightarrow \infty} \frac{\log \#C_\Gamma(\langle m_q \rangle, c_q)}{\text{vol}(m_q)} \geq 0$$

where the supremum is taken over all sequences satisfying the above conditions

h_Γ is upper semi-continuous on Π_Γ

8 Convex functions

$f : \mathbb{R}^n \rightarrow [-\infty, \infty]$ convex.

$\text{dom } f := \{\mathbf{x} \in \mathbb{R}^m : f(\mathbf{x}) < \infty\}$

f proper if $f : \mathbb{R}^n \rightarrow \bar{\mathbb{R}} := (-\infty, \infty]$ and $f \not\equiv \infty$

f closed if f is lower semi-continuous.

\mathbf{q} subgradient: $f(\mathbf{x}) \geq f(\mathbf{u}) + \mathbf{q}^\top (\mathbf{x} - \mathbf{u}) \forall \mathbf{x}$

$\partial f(\mathbf{u}) \subset \mathbb{R}^n$ the subset of subgradients of f at \mathbf{u}

ASSUMPTION: f is proper and closed

$\partial f(\mathbf{u})$ is a closed nonempty set for each $\mathbf{u} \in \text{ri dom } f$

f is differentiable at $\mathbf{u} \iff \partial f(\mathbf{u}) = \{\nabla f(\mathbf{u})\}$

$\text{diff } f$ - the set of differentiability points of f

∇f continuous on $\text{diff } f$ and $\overline{\text{diff } f} \supseteq \text{dom } f$

The conjugate, (Legendre transform) f^* defined:

$f^*(\mathbf{y}) := \sup_{\mathbf{x} \in \mathbb{R}^n} \mathbf{x}^\top \mathbf{y} - f(\mathbf{x})$ for each $\mathbf{y} \in \mathbb{R}^m$

f^* is a proper closed function and $f^{**} = f$

9 P_Γ^* and color density entropy

Thm 1: $h_\Gamma(p) \leq -P_\Gamma^*(p) \forall p \in \Pi_\Gamma$.

$$P_\Gamma(u) = \max_{p \in \Pi_\Gamma} (p^\top u + h_\Gamma(p)), u \in \mathbb{R}^n$$

$$\Pi_\Gamma(u) := \arg \max_{p \in \Pi_\Gamma} (p^\top u + h_\Gamma(p)) = \{p \in \Pi_\Gamma : P_\Gamma(u) = p^\top u + h_\Gamma(p)\}$$

For each $p \in \Pi_\Gamma(u)$, $h_\Gamma(p) = -P_\Gamma^*(p)$.

$$\Pi_\Gamma(u) \subseteq \partial P_\Gamma(u).$$

$$u \in \text{diff } P_\Gamma \Rightarrow \Pi_\Gamma(u) = \{\nabla P_\Gamma(u)\}.$$

Therefore $\partial P_\Gamma(\text{diff } P_\Gamma) \subseteq \Pi_\Gamma$.

$$S(u), u \in \mathbb{R}^n \setminus \text{diff } P_\Gamma$$

are all the limits of sequences

$$\nabla P_\Gamma(u_i), u_i \in \text{diff } P_\Gamma \text{ and } u_i \rightarrow u.$$

Then $S(u) \subseteq \Pi_\Gamma(u)$.

$$\text{conv } \Pi_\Gamma(u) = \text{conv } S(u) = \partial P_\Gamma(u).$$

$$\partial P_\Gamma(\mathbb{R}^n) \subseteq \text{conv } \Pi_\Gamma \subseteq \Pi_n.$$

$$\text{conv } \Pi_\Gamma = \text{dom } P_\Gamma^*.$$

10 Outline of proof

From the definitions of $P_\Gamma(\mathbf{u})$, \mathbf{p} , $h_\Gamma(\mathbf{p}) :=$
 $\sup_{\mathbf{m}_q, \mathbf{c}_q} \limsup_{q \rightarrow \infty} \frac{\log \#C_\Gamma(\langle \mathbf{m}_q \rangle, \mathbf{c}_q)}{\text{vol}(\mathbf{m}_q)} \geq 0$

$$P_\Gamma(\mathbf{u}) \geq \mathbf{p}^\top \mathbf{u} + h_\Gamma(\mathbf{p}) \Rightarrow$$

$$P_\Gamma(\mathbf{u}) \geq \sup_{\mathbf{p} \in \Pi_\Gamma} \mathbf{p}^\top \mathbf{u} + h_\Gamma(\mathbf{p}) \Rightarrow$$

$$-h_\Gamma(\mathbf{p}) \geq P_\Gamma^*(\mathbf{p}) \Rightarrow \Pi_\Gamma \subseteq \text{dom } P_\Gamma^*$$

$$C(\mathbf{m}, \mathbf{u}) :=$$

$$\arg \max_{\mathbf{c} \in \Pi_n(\text{vol}(\mathbf{m}))} \#C_\Gamma(\langle \mathbf{m} \rangle, \mathbf{c}) e^{\mathbf{c}^\top \mathbf{u}}$$

$$Z_\Gamma(\mathbf{m}, \mathbf{u}) =$$

$$O(\text{vol}(\mathbf{m})^{n-1}) \#C_\Gamma(\langle \mathbf{m} \rangle, \mathbf{c}(\mathbf{m}, \mathbf{u})) e^{\mathbf{c}(\mathbf{m}, \mathbf{u})^\top \mathbf{u}}$$

Let $\mathbf{m}_q \rightarrow \infty$ s.t. $\frac{\mathbf{c}(\mathbf{m}_q, \mathbf{u})}{\text{vol}(\mathbf{m}_q)} \rightarrow \mathbf{p}(\mathbf{u}) \Rightarrow P_\Gamma(\mathbf{u}) \leq$

$$\mathbf{p}(\mathbf{u})^\top \mathbf{u} + \limsup_{q \rightarrow \infty} \frac{\log \#C_\Gamma(\langle \mathbf{m}_q \rangle, \mathbf{c}(\mathbf{m}_q, \mathbf{u}))}{\text{vol}(\mathbf{m}_q)} \leq$$

$$\mathbf{p}(\mathbf{u})^\top \mathbf{u} + h_\Gamma(\mathbf{p}(\mathbf{u}))$$

For $\mathbf{p} \in \Pi_\Gamma(\mathbf{u})$ use maximal characterization

$$P_\Gamma(\mathbf{u} + \mathbf{v}) \geq \mathbf{p}^\top (\mathbf{u} + \mathbf{v}) + h_\Gamma(\mathbf{p}) = \mathbf{p}^\top \mathbf{v} + P_\Gamma(\mathbf{u})$$

So $\mathbf{p} \in \partial P_\Gamma(\mathbf{u}) \Rightarrow \Pi_\Gamma(\mathbf{u}) \subseteq \partial P_\Gamma(\mathbf{u}) \Rightarrow$

$$\mathbf{u} \in \text{diff } P_\Gamma \Rightarrow \Pi_\Gamma(\mathbf{u}) = \{\nabla P_\Gamma(\mathbf{u})\}$$

11 First order phase transition

Claim: For $\mathbf{u} \in \mathbb{R}^n$ each $\mathbf{p} \in \Pi_{\Gamma}(\mathbf{u})$ is the set of possible density of n colors in an allowable configurations from $C_{\Gamma}(\mathbb{Z}^d)$ with the potential \mathbf{u} .

For $\mathbf{u} \in \text{diff } P_{\Gamma}$ $\mathbf{p}(\mathbf{u}) = \nabla P_{\Gamma}(\mathbf{u})$ is a unique density.

Claim: Any point of nondifferentiability of P_{Γ} is a point of the phase transition.

Proof Let $\mathbf{u} \in \mathbb{R}^n \setminus \text{diff } P_{\Gamma}$ Then ∂P_{Γ} consists of more than one point. **Thm 1** yields that

$\partial P_{\Gamma}(\mathbf{u}) = \text{conv } S(\mathbf{u}) \subseteq \Pi_{\Gamma}(\mathbf{u})$. $S(\mathbf{u})$ consists of more than one point. Hence $\Pi_{\Gamma}(\mathbf{u})$ consists of more than one density for \mathbf{u} .

$\mathbf{u} \in \mathbb{R}^n \setminus \text{diff } P_{\Gamma}$ is called a point of **phase transition**, or a phase transition point of the **first order**.

12 Ergodic Notions

$C_\Gamma(\mathbb{Z}^d)$ -a compact metric space.

It is invariant under the shifts

$$\sigma_i : C_\Gamma(\mathbb{Z}^d) \rightarrow C_\Gamma(\mathbb{Z}^d), i = 1, \dots, d$$

$\sigma_i(\phi)$ is obtained by shifting the allowable configuration $\phi \in C_\Gamma(\mathbb{Z}^d)$ using the transformation $\mathbf{x} \mapsto \mathbf{x} - \mathbf{e}_i$.

Let \mathcal{M}_Γ be the compact set of invariant measures on $C_\Gamma(\mathbb{Z}^d)$ with respect to $\sigma_i, i = 1, \dots, d$.

$h_\Gamma(\mu)$ -Kolmogorov-Sinai entropy for $\mu \in \mathcal{M}_\Gamma$

$$h_\Gamma(\mu) = \lim_{m \rightarrow \infty} \frac{1}{(2m+1)^d}$$

$$H_\mu(\bigvee_{-m \leq i_1, \dots, i_d \leq m} \sigma_1^{i_1} \dots \sigma_d^{i_d} \mathcal{A})$$

where $\mathcal{A} = \{A_1, \dots, A_n\}$

a cylinder partition of $C_\Gamma(\mathbb{Z}^d)$.

A_i - the set of all configurations $\phi \in C_\Gamma(\mathbb{Z}^d)$ s.t.

$\mathbf{0} \in \mathbb{Z}^d$ colored by color i in ϕ .

13 The maximum principle

$f_{\mathbf{u}} : C_{\Gamma} \rightarrow \mathbb{R}$ be given by

$f_{\mathbf{u}}(\phi) = u_i$ for $\phi \in A_i$, $\mathbf{u} = (u_1, \dots, u_n)$.

$P_{\Gamma}(\mathbf{u}) = \max_{\mu \in \mathcal{M}_{\Gamma}} h_{\Gamma}(\mu) + \int f_{\mathbf{u}}(x) d\mu(x)$

$\mu_{\mathbf{u}} \in \mathcal{M}_{\Gamma}$ is maximal if

$P_{\Gamma}(\mathbf{u}) = h_{\Gamma}(\mu) + \int f_{\mathbf{u}}(x) d\mu(x)$

u -ergodic phase transition

if there are at least two maximal $\mu_{\mathbf{u}}$ measures

Conjecture If $\mathbf{u} \in \mathbb{R}^n \setminus \text{diff } P_{\Gamma}$ then \mathbf{u} is an ergodic phase transition

Special case studied case in the literature $\mathbf{u} = \mathbf{0}$:

The entropy

$$\begin{aligned} h_{\Gamma} &= P_{\Gamma}(\mathbf{0}) = \\ \max_{\mathbf{p} \in \Pi_{\Gamma}} h_{\Gamma}(\mathbf{p}) &= \\ \max_{\mu \in \mathcal{M}_{\Gamma}} h_{\Gamma}(\mu) \end{aligned}$$

14 d -Dimensional Monomer-Dimers

Dimer: (\mathbf{i}, \mathbf{j}) , $\mathbf{j} = \mathbf{i} + \mathbf{e}_k \in \mathbb{Z}^d$.

any partition of \mathbb{Z}^d to dimers (1-factor).

Monomer: occupies $\mathbf{i} \in \mathbb{Z}^d$.

any partition of \mathbb{Z}^d to monomer-dimers

is 1-factor of a subset of \mathbb{Z}^d .

Dimer and Monomer-Dimer are SOFT

$$0 = \tilde{h}_1 \leq \tilde{h}_2 \leq \dots \leq \tilde{h}_d \leq \dots (\text{dimers})$$

$$\log \frac{1 + \sqrt{5}}{2} = h_1 \leq h_2 \leq \dots \leq h_d \leq \dots$$

(monomer – dimer)

Fisher, Kasteleyn and Temperley 61

$$\tilde{h}_2 = \frac{1}{\pi} \sum_{i=0}^{\infty} \frac{(-1)^i}{(2i+1)^2} = 0.29156090\dots$$

15 Hammersley's results

Hammersley in 60's studied extensively the monomer-dimer model. He showed $\Pi_{\Gamma} = \Pi_{d+1}$ for d -dimensional model

$$p = (p_1, \dots, p_d, p_{d+1})$$

p_i -the dimer density in e_i -direction $i = 1, \dots, d$

p_{d+1} -the monomer density Hammersley studied

$p := p_1 + \dots + p_d$ -the total dimer density

$h_d(p)$ -the p -dimer density in \mathbb{Z}^d , $p \in [0, 1]$

He showed $h_d(p)$ -concave continuous function on $[0, 1]$

Heilmann and Lieb 72: $h_d(p)$ analytic on $(0, 1)$

No phase transition in parameter $p \in (0, 1)$

16 The Graphs for $h_2(p)$

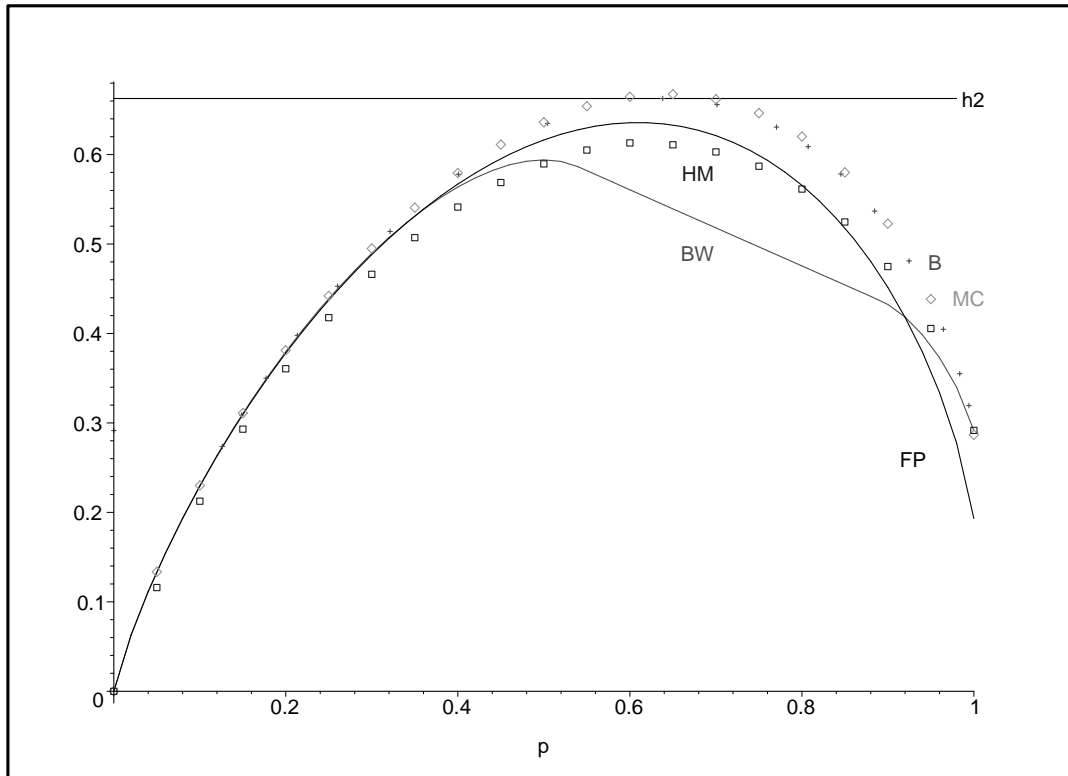


Figure 1: HM is the lower bound of Hammersley-Menon, BW is the lower bound of Bondy-Welsh, FP is the lower bound of Friedland-Peled, MC is the Monte Carlo estimate of Hammersley-Menon, B are Baxter's estimates, and h2 is the true value of $h_2 = \max h_2(p)$.

17 Graph estimates for $h_2(p)$

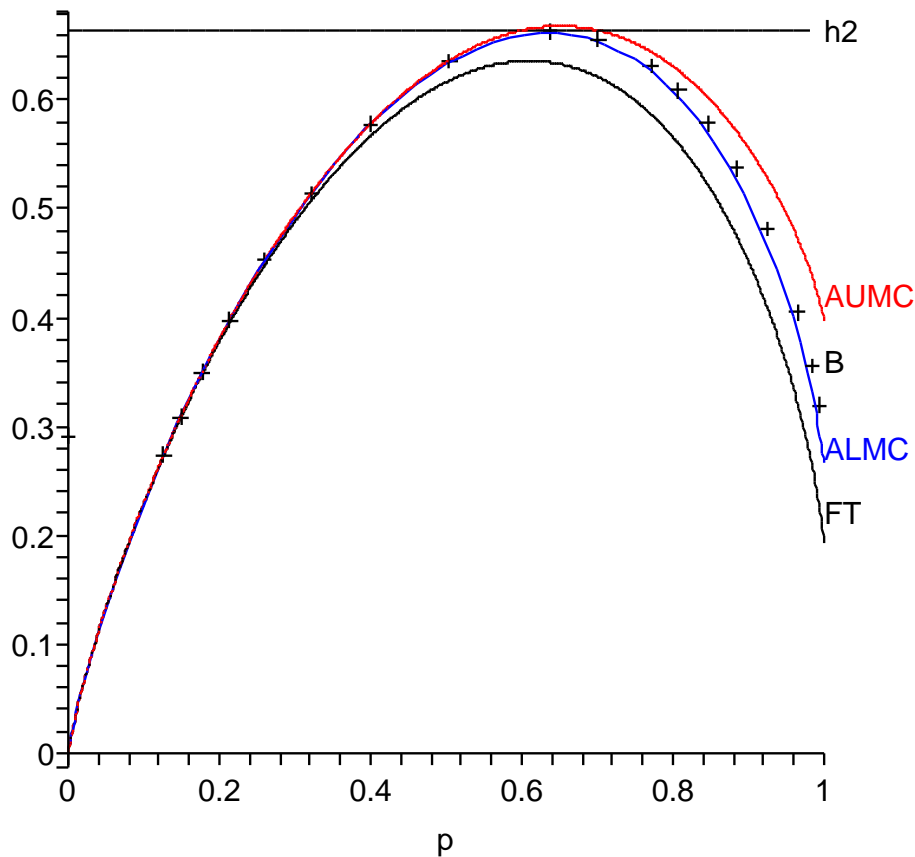


Figure 2: Monomer-dimer tiling of the **2**-dimensional grid: entropy as a function of dimer density. FT is the Friedland-Tverberg lower bound, h_2 is the true monomer-dimer entropy. B are Baxter's computed values. ALMC is the Asymptotic Lower Matching Conjecture. AUMC is the entropy of a countable union of $K_{4,4}$, conjectured to be an upper bound by the Asymptotic Upper Matching Conjecture.

18 Friendly colorings

Thm 1 implies:

For any Potts model $h_{\Gamma}(\cdot) : \Pi_{\Gamma} \rightarrow \mathbb{R}_+$ is concave on every convex subset of $\Pi_{\Gamma}(\mathbb{R}^n)$.

To get the exact analog of Hammersley's result

$\Gamma = (\Gamma_1, \dots, \Gamma_d)$ on $\langle n \rangle$

$\mathcal{F} = \cup_{\mathbf{m} \in \mathbb{N}^d} \tilde{\mathcal{C}}_{\Gamma}(\langle \mathbf{m} \rangle)$, where

$\tilde{\mathcal{C}}_{\Gamma}(\langle \mathbf{m} \rangle) \subseteq \mathcal{C}_{\Gamma}(\langle \mathbf{m} \rangle)$ for each $\mathbf{m} \in \mathbb{N}^d$, **friendly**: if whenever a box $\langle \mathbf{m} \rangle$ is cut in two and each part is colored by a coloring in \mathcal{F} , the combined coloring is in \mathcal{F} .

Γ **friendly** if there exist a friendly set

$\mathcal{F} = \cup_{\mathbf{m} \in \mathbb{N}^d} \tilde{\mathcal{C}}_{\Gamma}(\langle \mathbf{m} \rangle)$ and a constant vector $\mathbf{b} \in \mathbb{N}^d$ such that if any box $\langle \mathbf{m} \rangle$ is padded with an envelope of width b_i in the direction of \mathbf{e}_i , then each Γ -allowed coloring of $\langle \mathbf{m} \rangle$ can be extended in the padded part to a coloring in \mathcal{F} .

19 Examples of friendly colorings

Γ has a friendly color $f \in \langle n \rangle$, i.e., for each $i \in \langle d \rangle$
 $(f, j), (j, f) \in \Gamma_i$ for all $j \in \langle n \rangle$

Then $\tilde{C}_\Gamma(\mathbf{m})$ are Γ -allowed colorings of $\langle \mathbf{m} \rangle$ whose
boundary points are colored with f

Hard-core model: $\Gamma_i = \{(1, 1), (1, 2), (2, 1)\}$, has
friendly color $f = 1$.

Γ associated with the monomer-dimer covering

$\tilde{C}_\Gamma(\langle \mathbf{m} \rangle)$ the set of tilings of $\langle \mathbf{m} \rangle$ by monomers and
dimers, i.e., the coverings in which no dimer protrudes out of
 $\langle \mathbf{m} \rangle$, as in Hammersley

20 P_{Γ}^* for friendly colorings

Thm 2: Let $\Gamma = (\Gamma_1, \dots, \Gamma_d)$ be a friendly coloring digraph. Then

- (a) Π_{Γ} is convex. Hence $\Pi_{\Gamma} = \text{dom } P_{\Gamma}^*$.
- (b) $h_{\Gamma}(\cdot) : \Pi_{\Gamma} \rightarrow \mathbb{R}_+$ is concave.
- (c) For each $\mathbf{u} \in \mathbb{R}^n$, $\Pi_{\Gamma}(\mathbf{u}) = \partial P_{\Gamma}(\mathbf{u})$.
- (d) For each $\mathbf{u} \in \mathbb{R}^n$, $h_{\Gamma}(\cdot)$ is an affine function on $\partial P_{\Gamma}(\mathbf{u})$.
- (e) $h_{\Gamma}(\mathbf{p}) = -P_{\Gamma}^*(\mathbf{p})$ for each $\mathbf{p} \in \Pi_{\Gamma}$.

21 Outline of proof

(a). Let $\alpha \in \tilde{C}_\Gamma(\langle m \rangle)$,

$c(\alpha) = (c_1, \dots, c_n) \in \Pi_n(\text{vol}(m))$ color frequency vector of α , and $p := \frac{1}{\text{vol}(m)} c(\alpha)$.

For $k = (k_1, \dots, k_d) \in \mathbb{N}^d$ let

$k \cdot m := (k_1 m_1, \dots, k_d m_d)$. View $\langle k \cdot m \rangle$ as a box composed of $\text{vol}(k)$ boxes isomorphic to $\langle m \rangle$ color each box by α obtaining a coloring $\alpha(k \cdot m) \in \tilde{C}_\Gamma(k \cdot m)$.

Clearly $p = \frac{1}{\text{vol}(k \cdot m)} c(\alpha(k \cdot m))$. Choose $k_q \rightarrow \infty$ to deduce $p \in \Pi_\Gamma$.

Let $\beta \in \tilde{C}_\Gamma(\langle n \rangle)$. So $q := \frac{1}{\text{vol}(n)} c(\beta) \in \Pi_\Gamma$.

Claim: For $i, j \in \mathbb{N}$ $\frac{i}{i+j} p + \frac{j}{i+j} q \in \Pi_\Gamma$.

Let $\alpha(n \cdot m), \beta(m \cdot n) \in \tilde{C}_\Gamma(n \cdot m)$ defined as above. Let

$k := (m_1 n_1, \dots, m_{d-1} n_{d-1}, (i+j) m_d n_d)$

view box $\langle k \rangle$ composed of $i+j$ boxes isomorphic to $\langle m \cdot n \rangle$ aligned side-by-side along the direction of e_d .

Color the first i of these boxes by $\alpha(m \cdot n)$ and the last j by $\beta(n \cdot m)$, to get $\gamma \in \tilde{C}_\Gamma(\langle k \rangle)$ with

$\frac{1}{\text{vol}(\mathbf{k})} \mathbf{c}(\gamma) = \frac{i}{i+j} \mathbf{p} + \frac{j}{i+j} \mathbf{q}$. Hence

$\frac{i}{i+j} \mathbf{p} + \frac{j}{i+j} \mathbf{q} \in \Pi_\Gamma$. Since Π_Γ is closed
 $a\mathbf{p} + (1-a)\mathbf{q} \in \Pi_\Gamma$ for all $a \in [0, 1]$.

Let $\tilde{\Pi}_\Gamma$ be the convex hull of $\frac{1}{\text{vol}(\mathbf{m})} \mathbf{c}(\alpha)$ for some \mathbf{m} and
some $\alpha \in \tilde{C}_\Gamma(\langle \mathbf{m} \rangle)$. So $\tilde{\Pi}_\Gamma \subseteq \Pi_\Gamma$.

The padding part of definition of Γ friendly implies

$$\tilde{\Pi}_\Gamma \subseteq \Pi_\Gamma \subseteq \text{cl } \tilde{\Pi}_\Gamma \Rightarrow \Pi_\Gamma = \text{cl } \tilde{\Pi}_\Gamma$$

Equality $\Pi_\Gamma = \text{dom } P_\Gamma^*$ follows from last part of Thm 1.

(b) The padding part of definition of Γ friendly implies

For $\mathbf{p}, \mathbf{q} \in \Pi_\Gamma, \varepsilon > 0 \exists$

$\mathbf{m}_q := (m_{1,q}, \dots, m_{d,q}), \mathbf{n}_q :=$

$(n_{1,q}, \dots, n_{d,q}) \in \mathbb{N}^d, q \in \mathbb{N}, \mathbf{m}_q, \mathbf{n}_q \rightarrow \infty$ s.t.

$$\tilde{C}_\Gamma(\langle \mathbf{m}_q \rangle, \mathbf{c}_q), \tilde{C}_\Gamma(\langle \mathbf{n}_q \rangle, \mathbf{d}_q) \neq \emptyset, q \in \mathbb{N},$$

$$\lim_{\mathbf{m}_q \rightarrow \infty} \frac{1}{\text{vol}(\mathbf{m}_q)} \mathbf{c}_q = \mathbf{p}, \lim_{\mathbf{n}_q \rightarrow \infty} \frac{1}{\text{vol}(\mathbf{n}_q)} \mathbf{d}_q = \mathbf{q}$$

$$\lim_{q \rightarrow \infty} \frac{\log \# \tilde{C}_\Gamma(\langle \mathbf{m}_q \rangle, \mathbf{c}_q)}{\text{vol}(\mathbf{m}_q)} \geq h_\Gamma(\mathbf{p}) - \varepsilon,$$

$$\lim_{q \rightarrow \infty} \frac{\log \# \tilde{C}_\Gamma(\langle \mathbf{n}_q \rangle, \mathbf{d}_q)}{\text{vol}(\mathbf{n}_q)} \geq h_\Gamma(\mathbf{q}) - \varepsilon.$$

Observation that for any

$\mathbf{m}, \mathbf{n} \in \mathbb{N}^d, \mathbf{c} \in \Pi_n(\text{vol}(\mathbf{m}))$:

$$\#\tilde{C}_\Gamma(\langle \mathbf{n} \cdot \mathbf{m} \rangle, \text{vol}(\mathbf{n})\mathbf{c}) \geq (\#\tilde{C}_\Gamma(\langle \mathbf{m} \rangle, \mathbf{c}))^{\text{vol}(\mathbf{n})}$$

yields: For $i, j \in \mathbb{N}$

$$h_\Gamma\left(\frac{i}{i+j}\mathbf{p} + \frac{j}{i+j}\mathbf{q}\right) \geq \frac{i}{i+j}h_\Gamma(\mathbf{p}) + \frac{j}{i+j}h_\Gamma(\mathbf{q}) - \varepsilon$$

which proves the concavity of h_Γ .

(c-d): Let $\mathbf{u} \in \text{diff } P_\Gamma$. Then

$\Pi_\Gamma(\mathbf{u}) = \{\nabla P_\Gamma(\mathbf{u})\} = \partial P_\Gamma(\mathbf{u})$ and (c-d) trivially hold.

Recall $S(\mathbf{u}) \subseteq \Pi_\Gamma(\mathbf{u})$,

$$\text{conv } S(\mathbf{u}) = \partial P_\Gamma(\mathbf{u}) \supseteq \Pi_\Gamma(\mathbf{u})$$

Let $\mathbf{p}_i \in S(\mathbf{u}), i = 1, \dots, j$. So

$$P_\Gamma(\mathbf{u}) = \mathbf{p}_i^\top \mathbf{u} + h_\Gamma(\mathbf{p}_i), i = 1, \dots, j$$

Since Π_Γ convex, for $\mathbf{a} = (a_1, \dots, a_j) \in \Pi_j$

$\mathbf{p} := \sum_{i=1}^j a_i \mathbf{p}_i \in \Pi_\Gamma$. As h_Γ concave

$$P_\Gamma(\mathbf{u}) = \sum_{i=1}^j a_i \mathbf{p}_i^\top \mathbf{u} + h_\Gamma(\mathbf{p}_i) \leq \mathbf{p}^\top \mathbf{u} + h_\Gamma(\mathbf{p})$$

The maximal characterization of $P_\Gamma(\mathbf{u})$ implies

$$P_\Gamma(\mathbf{u}) = \mathbf{p}^\top \mathbf{u} + h_\Gamma(\mathbf{p}). \text{ So } \mathbf{p} \in \Pi_\Gamma(\mathbf{u}) \text{ and}$$

$$h_\Gamma(\mathbf{p}) = \sum_{i=1}^j a_i h_\Gamma(\mathbf{p}_i).$$

(e) Follows from Thm 1 and extra arguments using convexity of P_Γ^*

22 Reduction of one parameter

$$P_{\Gamma}(\mathbf{u}) = t + P_{\Gamma}(\mathbf{u} - t\mathbf{1}) \Rightarrow \partial P_{\Gamma}(\mathbf{u}) \in \Pi_n$$

It is enough to compute

$$\hat{P}_{\Gamma}(\hat{\mathbf{u}}) := P_{\Gamma}(\hat{\mathbf{u}}), \hat{\mathbf{u}} = (u_1, \dots, u_{n-1}, 0)$$

Hard core model: $\hat{P}_{\Gamma}(t)$ depends on the energy $t \in \mathbb{R}$.

(It is known that for $d \geq 2$ hard core model has phase transition)

For the dimer problem the pressure $P_d(\mathbf{v})$ depends on $\mathbf{v} = (v_1, \dots, v_d)$, where v_i is the energy of the dimer in the direction \mathbf{e}_i , $i = 1, \dots$. (Non-isotropic model)

Dimer isotropic model in \mathbb{Z}^d : pressure $P_d(v)$, where v is the energy of the dimer in any direction.

(Standard model-No phase transition for $v \in \mathbb{R}$)

23 Computation of pressure

Using the scaled transfer matrices on the torus

$T(\mathbf{m}')$, $\mathbf{m}' = (m_1, \dots, m_{d-1})$ as in Friedland-Peled 2005 [6].

Assume for simplicity $d = 2, \Gamma = (\Gamma_1, \Gamma_2)$, where Γ_1 symmetric digraph. Let Δ transfer digraph induced by Γ_2 between the allowable Γ_1 coloring of the circle $T(\mathbf{m})$.

Then $V := C_{\Gamma_1, \text{per}}(\mathbf{m})$ are the set of vertices of $\Delta(\mathbf{m})$. For $\alpha, \beta \in C_{\Gamma_1, \text{per}}(\mathbf{m})$ the directed edge (α, β) is in $\Delta(\mathbf{m})$ iff the configuration $[(\alpha, \beta)]$ is an allowable configuration on $C_{\Gamma}((\mathbf{m}, 2))$. Adjacency matrix $D(\Delta(\mathbf{m})) = (d_{\alpha\beta})_{\alpha, \beta \in C_{\Gamma_1, \text{per}}(\mathbf{m})}$ is $N \times N$ matrix, where $N := \#C_{\Gamma_1, \text{per}}(\mathbf{m})$. One dimensional SOFT is $C_{\Gamma}(T(\mathbf{m}) \times \mathbb{Z})$: all Γ allowable coloring of the infinite torus in the direction \mathbf{e}_2 with the basis $T(\mathbf{m})$. The pressure corresponding to this one dimensional SOFT is denoted by $\tilde{P}_{\Delta(\mathbf{m})}(\mathbf{u})$. Its formula:

Let $\tilde{D}(\Delta(m), \mathbf{u}) = (\tilde{d}_{\alpha\beta}(\mathbf{u}))_{\alpha, \beta \in C_{\Gamma_1, \text{per}}(m)}$

$$\tilde{d}_{\alpha\beta}(\mathbf{u}) = d_{\alpha\beta} e^{\frac{1}{2}(c(\alpha) + c(\beta))^\top \mathbf{u}}$$

Then $\tilde{P}_\Delta(\mathbf{u}) := \frac{\theta(\mathbf{u}, m)}{m}$,

$$\theta(\mathbf{u}, m) := \log \rho(\tilde{D}(\Delta(m), \mathbf{u}))$$

(We divide $\log \rho(\tilde{D}(\Delta, \mathbf{u}))$ by m , to have

$$\tilde{P}_\Delta(\mathbf{u} + t\mathbf{1}) = \tilde{P}_\Delta(\mathbf{u}) + t \quad \text{for any } t \in \mathbb{R}$$

Main inequalities

$$\frac{1}{p}(\theta(\mathbf{u}, p + 2q) - \theta(\mathbf{u}, 2q)) \leq P_\Gamma(\mathbf{u})$$

$$\leq \frac{1}{2m}(\theta(\mathbf{u}, 2m))$$

for any $m, p \geq 1$ and $q \geq 0$.

24 Automorphism Subgroups

$A = (a_{ij})_1^N$ nonnegative matrix $\mathcal{A}(A) :=$
 $\{\pi \in S_N : a_{\pi(i)\pi(j)} = a_{ij}, i, j \in \langle N \rangle\}$

Let $G \leq \mathcal{A}(A)$,

$\mathcal{O}(G) := \langle N \rangle / G$,

$M = \#\mathcal{O}(G)$

$\hat{A} = (\hat{a}_{\alpha\beta})_{\alpha, \beta \in \mathcal{O}(G)}$, $\hat{a}_{\alpha\beta} =: \sum_{j \in \beta} a_{ij}$, $i \in \alpha$,

$\rho(A) = \rho(\hat{A})$,

If $A = A^T$ then \hat{A} symmetric for

$\langle x, y \rangle = \sum_{\alpha \in \mathcal{O}(G)} (\#\alpha) x_\alpha y_\alpha$.

$M \geq N/\#G$,

In our computations $M \sim N/\#G$

Using these tools we confirmed Baxter's computations with nine digits of precision of $P_2(v)$ and of $h_2(p)$.

We also computed the non-isotropic $P_2((v_1, v_2))$.

References

- [1] V. I. Arnold, *Mathematical Methods of Classical Mechanics*, Springer, New York, 1978.
- [2] R. J. Baxter, Dimers on a rectangular lattice, *J. Math. Phys.* 9 (1968), 650–654.
- [3] S. Friedland, On the entropy of Z-d subshifts of finite type, *Linear Algebra Appl.* 252 (1997), 199–220.
- [4] S. Friedland, Multi-dimensional capacity, pressure and Hausdorff dimension, in *Mathematical System Theory in Biology, Communication, Computation and Finance*, edited by J. Rosenthal and D. Gilliam, IMA Vol. Ser. 134, Springer, New York, 2003, 183–222.
- [5] S. Friedland, E. Krop, P. H. Lundow and K. Markström, Computational validations of the asymptotic matching conjectures, submitted.
- [6] S. Friedland and U. N. Peled, Theory of Computation of Multidimensional Entropy with an Application to the Monomer-Dimer Problem, *Advances of Applied Math.* 34(2005), 486-522.

- [7] F. R. Gantmacher, *The Theory of Matrices*, Vol. II, Chelsea Publ. Co., New York 1959.
- [8] J. M. Hammersley, Existence theorems and Monte Carlo methods for the monomer-dimer problem, in *Research papers in statistics: Festschrift for J. Neyman*, edited by F.N. David, Wiley, London, 1966, 125–146.
- [9] O. J. Heilmann and E. H. Lieb, Theory of monomer-dimer systems, *Comm. Math. Phys.* 25 (1972), 190–232; Errata 27 (1972), 166.
- [10] E. Ising, Beitrag zur Theory des Ferromagnetismus, *Z. Physik* 31 (1925), 253–?.
- [11] P.W. Kasteleyn, The statistics of dimers on a lattice, *Physica* 27 (1961), 1209–1225.
- [12] J. F. C. Kingman, A convexity property of positive matrices. *Quart. J. Math. Oxford Ser. (2)* 12 (1961), 283–284.
- [13] L. Onsager, Crystal statistics, I. A two-dimensional model with an order-disorder transition, *Phys. Review* 65 (1944), 117–?

- [14] R.B. Potts, ?, *Proc. Cambridge Phil. Soc.* 48 (1952), 106–?
- [15] R. T. Rockafeller, *Convex Analysis*, Princeton Univ. Press 1970.
- [16] H. N. V. Temperley and M. E. Fisher, Dimer problem in statistical mechanics—an exact result, *Phil. Mag.* (8) 6 (1961), 1061–1063.
- [17] C. J. Thompson, *Mathematical Statistical Mechanics*, Princeton Univ. Press, 1972.