Theoretical and computational methods in statistical mechanics

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## Overview

- Motivation: Ising model
- Subshifts of Finite Type
- Pressure P<sub>Γ</sub>
- Density points and density entropy
- Convex functions
- *P*<sup>\*</sup><sub>Γ</sub> and color density entropy
- First order phase transition
- d-Dimensional Monomer-Dimers
- Friendly colorings
- Computation of pressure

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#### Figure: Uri Natan Peled, Photo - December 2006

Uri was born in Haifa, Israel, in 1944. Education:

Hebrew University, Mathematics-Physics, B.Sc., 1965. Weizmann Institute of Science, Physics, M.Sc., 1967 University of Waterloo, Mathematics, Ph.D., 1976 University of Toronto, Postdoc in Mathematics, 1976–78 Appointments:

1978–82, Assistant Professor, Columbia University 1982–91, Associate Professor, University of Illinois at Chicago 1991–2009, Professor, University of Illinois at Chicago Areas of research: Graphs, combinatorial optimization, boolean functions.

Uri published about 57 paper

Uri died September 6, 2009 after a long battle with brain tumor.

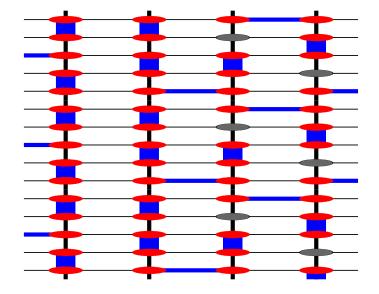


Figure: Matching on the two dimensional grid: Bipartite graph on 60 vertices, 101 edges, 24 dimers, 12 monomers

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## 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  $(\mathbf{i}, \mathbf{i} + \mathbf{e}_i)$  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:  $\frac{k}{T}E(\phi)$ 

# Motivation: Ising model - 1925

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$$d = 2, H = 0.$$

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# Subshifts of Finite Type-SOFT

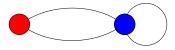
ALPHABET ON *n* LETTERS - COLORS.



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  $n = 2, < 2 >= \{1, 2\} = \{1, 0\} (2 \equiv 0).$ NO TWO 1's ARE NEIGHBORS.

## One dimensional SOFT

 $\Gamma \subseteq \langle n \rangle \times \langle n \rangle \text{ directed graph on } n \text{ vertices } C_{\Gamma}(\langle m \rangle) \text{-all } \Gamma$ allowable configurations of length m:  $\{a = a_1 \dots a_m = (a_i)_1^m : \langle m \rangle \rightarrow \langle n \rangle (a_i, a_{i+1}) \in \Gamma\}$  $C_{\Gamma}(\mathbb{Z}) \text{-all } \Gamma \text{ allowable configurations (tilings) on } \mathbb{Z}$ :  $\{a = (a_i)_{i \in \mathbb{Z}} : \mathbb{Z} \rightarrow \langle n \rangle, (a_i, a_{i+1}) \in \Gamma\}$ Hard core model:  $n = 2, \Gamma = \{\bullet \bullet, \bullet \bullet, \bullet \bullet\}$ 



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#### MD SOFT=Potts Models

Dimension  $d \ge 2$ . For  $\mathbf{m} \in \mathbb{N}^d$ ,  $\langle \mathbf{m} \rangle := \langle m_1 \rangle \times \ldots \times \langle m_d \rangle$ vol $(\mathbf{m}) := |m_1| \times \ldots \times |m_d|$ ,  $\Gamma := (\Gamma_1, \ldots, \Gamma_d)$ ,  $\Gamma_i \subset \langle n \rangle \times \langle n \rangle$  $C_{\Gamma}(\langle \mathbf{m} \rangle)$ -all  $\Gamma$  allowable configurations of  $\mathbf{m}$ :  $a = (a_i)_{i \in \langle \mathbf{m} \rangle} :< \mathbf{m} \rangle \rightarrow \langle n \rangle$  s.t.  $(a_i, a_{i+\mathbf{e}_j}) \in \Gamma_j$  if  $\mathbf{i}, \mathbf{i} + \mathbf{e}_j \in \langle \mathbf{m} \rangle$  $\mathbf{e}_j = (\delta_{1j}, \ldots, \delta_{dj}), j = 1, \ldots, d$ . Example:





### MD SOFT=Potts Models II

For  $\phi \in C_{\Gamma}(\langle \mathbf{m} \rangle)$  -  $\mathbf{c}(\phi) := (c_1(\phi), \dots, c_n(\phi))$ denotes coloring distribution of configuration  $\phi$  $c_i(\phi)$ -the number of times the particle *i* appears in  $\phi$  $\frac{1}{\operatorname{vol}(\mathbf{m})}\mathbf{c}(\phi) \in \Pi_n$  - coloring frequency of  $\phi$  $\Pi_n(\text{vol}(\mathbf{m})) \text{ all } \mathbf{c} \in \mathbb{Z}^n_+ \text{ s.t. } \frac{1}{\text{vol}(\mathbf{m})} \mathbf{c} \in \Pi_n$  $C_{\Gamma}(\langle \mathbf{m} \rangle, \mathbf{c})$  denotes all  $\phi \in C_{\Gamma}(\langle \mathbf{m} \rangle)$  with  $\mathbf{c}(\phi) = \mathbf{c}$ .  $C_{\Gamma,\text{per}}(\langle \mathbf{m} \rangle) \subseteq C_{\Gamma}(\langle \mathbf{m} \rangle)$ -m-periodic configurations  $C_{\Gamma}(\mathbb{Z}^d)$ -are- $\Gamma$  allowable configurations of  $\mathbb{Z}^d$ Assumption:  $C_{\Gamma}(\mathbb{Z}^d) \neq \emptyset$  $u_i \in \mathbb{R}$  energy of particle  $i \in \langle n \rangle$  $\mathbf{u} := (u_1, \ldots, u_n) \in \mathbb{R}^n$  energy vector  $E(\phi) = \mathbf{c}(\phi) \cdot \mathbf{u}$  Energy of configuration  $\phi$ Near neighbor interaction model, can be fit to the above noninteraction model by considering the coloring of the cube  $\langle (3, \ldots, 3) \rangle$  as one particle Similarly short range interaction model 

Grand partition function  $Z_{\Gamma}(\mathbf{m},\mathbf{u}) := \sum_{\phi \in C_{\Gamma}(\langle \mathbf{m} \rangle)} e^{\mathbf{c}(\phi) \cdot \mathbf{u}}$ log  $Z_{\Gamma}(\mathbf{m}, \mathbf{u})$  subadditive in each component of **m** and convex in **u**  $\frac{1}{vol(\mathbf{m})}\log Z_{\Gamma}(\mathbf{m},\mathbf{u})$  - average energy or pressure  $P_{\Gamma}(\mathbf{u}) := \lim_{\mathbf{m} \to \infty} \frac{1}{\operatorname{vol}(\mathbf{m})} \log Z_{\Gamma}(\mathbf{m}, \mathbf{u})$ **Pressure of \Gamma-SOFT.** (Pressure of the Potts model)  $h_{\Gamma} := P_{\Gamma}(\mathbf{0})$ -ENTROPY of  $\Gamma$ -SOFT  $P_{\Gamma}(\mathbf{u})$  is a convex Lipschitz function on  $\mathbb{R}^n$  $|P_{\Gamma}(\mathbf{u}) - P_{\Gamma}(\mathbf{v})| < ||\mathbf{u} - \mathbf{v}||_{\infty} := \max |u_i - v_i|$  $P_{\Gamma}(\mathbf{u} + t\mathbf{1}) = P_{\Gamma}(\mathbf{u}) + t$  $P_{\Gamma}$  has the following properties: Has subdifferential  $\partial P_{\Gamma}(\mathbf{u})$  for each  $\mathbf{u}$  $\partial P_{\Gamma}(\mathbf{u}) \subset \prod_{n}$  for each  $\mathbf{u}$ Has differentiable  $\nabla P_{\Gamma}(\mathbf{u})$  a.e.

 $\mathbf{p} \in \Pi_n$  density point of  $C_{\Gamma}(\mathbb{Z}^d)$  when there exist sequences of boxes  $\langle \mathbf{m}_q \rangle \subseteq \mathbb{N}^d$  and color distribution vectors  $\mathbf{c}_q \in \Pi_n(\operatorname{vol}(\mathbf{m}_q))$  $\mathbf{m}_q \to \infty$ ,  $C_{\Gamma}(\langle \mathbf{m}_q \rangle, \mathbf{c}_q) \neq \emptyset \quad \forall q \in \mathbb{N}$ , and  $\lim_{q \to \infty} \frac{\mathbf{c}_q}{\operatorname{vol}(\mathbf{m}_q)} = \mathbf{p}$  $\Pi_{\Gamma}$  the set of all density points of  $C_{\Gamma}(\mathbb{Z}^d)$  $\Pi_{\Gamma}$  is a closed set For  $\mathbf{p} \in \Pi_{\Gamma}$  the color density entropy  $h_{\Gamma}(\mathbf{p}) := \sup_{\mathbf{m}_q, \mathbf{c}_q} \limsup_{q \to \infty} \frac{\log \# C_{\Gamma}(\langle \mathbf{m}_q \rangle, \mathbf{c}_q)}{\operatorname{vol}(\mathbf{m}_q)} \geq 0$ where the supremum is taken over all sequences satisfying the above conditions

 $h_{\Gamma}$  is upper semi-continuous on  $\Pi_{\Gamma}$ 

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 $f : \mathbb{R}^n \to [-\infty, \infty]$  convex. dom  $f := \{\mathbf{x} \in \mathbb{R}^m : f(\mathbf{x}) < \infty\}$ f proper if  $f : \mathbb{R}^n \to \overline{\mathbb{R}} := (-\infty, \infty]$  and  $f \neq \infty$  f closed if f is lower semi-continuous.

**q** subgradient:  $f(\mathbf{x}) \ge f(\mathbf{u}) + \mathbf{q}^{\top}(\mathbf{x} - \mathbf{u}) \forall \mathbf{x} \partial f(\mathbf{u}) \subset \mathbb{R}^n$  the subset of subgradients of *f* at **u** ASSUMPTION: *f* is proper and closed  $\partial f(\mathbf{u})$  is a closed nonempty set for each  $\mathbf{u} \in \operatorname{ri} \operatorname{dom} f$  *f* is differentiable at  $\mathbf{u} \iff \partial f(\mathbf{u}) = \{\nabla f(\mathbf{u})\} \operatorname{diff} f$  - the set of differentiability points of *f*  $\nabla f$  continuous on diff *f* and  $\operatorname{diff} f \supseteq \operatorname{dom} f$ 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  $f^{**} = f$ 

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Thm 1: h_{\Gamma}(\mathbf{p}) \leq -P_{\Gamma}^*(\mathbf{p}) \forall \mathbf{p} \in \Pi_{\Gamma}.
P_{\Gamma}(\mathbf{u}) = \max_{\mathbf{p} \in \Pi_{\Gamma}}(\mathbf{p}^{\top}\mathbf{u} + h_{\Gamma}(\mathbf{p})), \mathbf{u} \in \mathbb{R}^{n}
\Pi_{\Gamma}(\mathbf{u}) := \arg \max_{\mathbf{p} \in \Pi_{\Gamma}} (\mathbf{p}^{\top} \mathbf{u} + h_{\Gamma}(\mathbf{p})) = \{ \mathbf{p} \in \Pi_{\Gamma} : P_{\Gamma}(\mathbf{u}) = \mathbf{p}^{\top} \mathbf{u} + h_{\Gamma}(\mathbf{p}) \}
For each \mathbf{p} \in \Pi_{\Gamma}(\mathbf{u}), h_{\Gamma}(\mathbf{p}) = -P_{\Gamma}^{*}(\mathbf{p}). \Pi_{\Gamma}(\mathbf{u}) \subseteq \partial P_{\Gamma}(\mathbf{u}).
\mathbf{u} \in \operatorname{diff} P_{\Gamma} \Rightarrow \Pi_{\Gamma}(\mathbf{u}) = \{\nabla P_{\Gamma}(\mathbf{u})\}.
Therefore \partial P_{\Gamma}(\operatorname{diff} P_{\Gamma}) \subset \Pi_{\Gamma}.
S(\mathbf{u}), \mathbf{u} \in \mathbb{R}^n \setminus \operatorname{diff} P_{\Gamma}-
are all the limits of sequences
\nabla P_{\Gamma}(\mathbf{u}_i), \mathbf{u}_i \in \operatorname{diff} P_{\Gamma} \operatorname{and} \mathbf{u}_i \to \mathbf{u}.
Then S(\mathbf{u}) \subset \Pi_{\Gamma}(\mathbf{u}).
conv \Pi_{\Gamma}(\mathbf{u}) = \operatorname{conv} S(\mathbf{u}) = \partial P_{\Gamma}(\mathbf{u}).
\partial P_{\Gamma}(\mathbb{R}^n) \subset \operatorname{conv} \Pi_{\Gamma} \subset \Pi_n.
conv \Pi_{\Gamma} = \operatorname{dom} P_{\Gamma}^*.
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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 nondifferentiabity of  $P_{\Gamma}$  is a point of the phase transition.

Proof Let  $\mathbf{u} \in \mathbb{R}^n \setminus \text{diff } P_{\Gamma}$  Then  $\partial P_{\Gamma}$  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.

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#### d-Dimensional Monomer-Dimers

Dimer: (**i**, **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

$$0 = ilde{h}_1 \leq ilde{h}_2 \leq ... \leq ilde{h}_d \leq ... ( ext{dimers})$$

$$\log \frac{1+\sqrt{5}}{2} = h_1 \le h_2 \le \dots \le h_d \le \dots$$
(monomer - dimer)

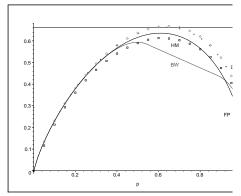
Fisher, Kasteleyn and Tempreley 61

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

Hammersley in 60's studied extensively the monomer-dimer model. He showed  $\Pi_{\Gamma} = \Pi_{d+1}$  for *d*-dimensional model  $\mathbf{p} = (p_1, \dots, p_d, p_{d+1})$  $p_i$ -the dimer density in  $\mathbf{e}_i$ -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]Heilman and Lieb 72:  $h_d(p)$  analytic on (0, 1)No phase transition in parameter  $p \in [0, 1)$ Au-Yang - Perk 84: Phase transition at dimers p = 1

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# The Graphs for $h_2(p)$



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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 b2 is the true value of  $h_2 = \max_2 n_2 n_2$ 

## Graph estimates for $h_2(p)$

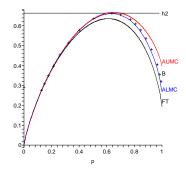


Figure 1: Monomer-dimer tiling of the 2-dimensional grid: entropy as a function of dimer density. FT is the Friedland-Tverbeg lower bound, h2 is the true monomer-dimer entropy. B are Baxter's computed values: ALMC is the Asymptotic Lower Matching Conjecture. AUMC is the entropy of a countable union of  $K_{4,4}$ , conjectured to be an upper bound by the Asymptotic Upper Matching Conjecture.

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#### Thm 1 implies:

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

To get the exact analog of Hammersley's result

 $\Gamma = (\Gamma_1, \ldots, \Gamma_d)$  on  $\langle n \rangle \mathcal{F} = \bigcup_{\mathbf{m} \in \mathbb{N}^d} \widetilde{C}_{\Gamma}(\langle \mathbf{m} \rangle)$ , where  $\widetilde{C}_{\Gamma}(\langle \mathbf{m} \rangle) \subseteq C_{\Gamma}(\langle \mathbf{m} \rangle)$ 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  $\mathcal{F}$ .  $\Gamma$  friendly if there exist a friendly set  $\mathcal{F} = \bigcup_{\mathbf{m} \in \mathbb{N}^d} \widetilde{C}_{\Gamma}(\langle \mathbf{m} \rangle)$  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  $\Gamma$ -allowed coloring of  $\langle \mathbf{m} \rangle$  can be extended in the padded part to a coloring in  $\mathcal{F}$ .

- Γ has a friendly color  $f \in \langle n \rangle$ , i.e., for each  $i \in \langle d \rangle$   $(f,j), (j,f) \in Γ_i$  for all  $j \in \langle n \rangle$
- Then  $C_{\Gamma}(\mathbf{m})$  are  $\Gamma$ -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.  $\Gamma$  associated with the monomer-dimer covering
- $\widetilde{C}_{\Gamma}(\langle \mathbf{m} \rangle)$  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

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

- **1**  $\Pi_{\Gamma}$  is convex. Hence  $\Pi_{\Gamma} = \operatorname{dom} P_{\Gamma}^*$ .
- 2  $h_{\Gamma}(\cdot) : \Pi_{\Gamma} \to \mathbb{R}_+$  is concave.
- **3** For each  $\mathbf{u} \in \mathbb{R}^n$ ,  $\Pi_{\Gamma}(\mathbf{u}) = \partial P_{\Gamma}(\mathbf{u})$ .
- For each  $\mathbf{u} \in \mathbb{R}^n$ ,  $h_{\Gamma}(\cdot)$  is an affine function on  $\partial P_{\Gamma}(\mathbf{u})$ .
- $h_{\Gamma}(\mathbf{p}) = -P_{\Gamma}^*(\mathbf{p})$  for each  $\mathbf{p} \in \Pi_{\Gamma}$ .

- $P_{\Gamma}(\mathbf{u}) = t + P_{\Gamma}(\mathbf{u} t\mathbf{1}) \Rightarrow \partial P_{\Gamma}(\mathbf{u}) \in \Pi_n$  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  $d \ge 2$  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  $v \in \mathbb{R}$ )

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Using the scaled transfer matrices on the torus  $T(\mathbf{m}'), \mathbf{m}' = (m_1, ..., m_{d-1})$  as in Friedland-Peled 2005 [3]. Assume for simplicity  $d = 2, \Gamma = (\Gamma_1, \Gamma_2)$ , where  $\Gamma_1$  symmetric digraph. Let  $\Delta$  transfer digraph induced by  $\Gamma_2$  between the allowable  $\Gamma_1$  coloring of the circle T(m). Then  $V := C_{\Gamma_1, \text{per}}(m)$  are the set of vertices of  $\Delta(m)$ . For  $\alpha, \beta \in C_{\Gamma_1, \text{per}}(m)$  the directed edge  $(\alpha, \beta)$  is in  $\Delta(m)$  iff the configuration  $[(\alpha, \beta)]$  is an allowable configuration on  $C_{\Gamma}((m, 2))$ . Adjacency matrix  $D(\Delta(m)) = (d_{\alpha\beta})_{\alpha,\beta\in C_{\Gamma_1,per}(m)}$  is  $N \times N$  matrix, where  $N := \#C_{\Gamma_1, \text{per}}(m)$ . One dimensional SOFT is  $C_{\Gamma}(T(m) \times \mathbb{Z})$ : all Γ allowable coloring of the infinite torus in the direction  $\mathbf{e}_2$  with the basis T(m). The pressure corresponding to this one dimensional SOFT is denoted by  $\tilde{P}_{\Delta(m)}(\mathbf{u})$ . Its formula:

Let  $\tilde{D}(\Delta(m), \mathbf{u}) = (\tilde{d}_{\alpha\beta}(\mathbf{u}))_{\alpha,\beta\in C_{\Gamma_1,per}(m)} \tilde{d}_{\alpha\beta}(\mathbf{u}) = d_{\alpha\beta}e^{\frac{1}{2}(\mathbf{c}(\alpha)+\mathbf{c}(\beta))^{\top}\mathbf{u}}$ 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  $\tilde{P}_{\Delta}(\mathbf{u}+t\mathbf{1}) = \tilde{P}_{\Delta}(\mathbf{u}) + t$  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  $q \geq 0$ .  $A = (a_{ij})_{1}^{N} \text{ nonnegative matrix}$   $\mathcal{A}(A) := \{\pi \in S_{N} : a_{\pi(i)\pi(j)} = a_{ij}, i, j \in \langle N \rangle\} \text{ Let}$   $G \leq \mathcal{A}(A), \mathcal{O}(G) := \langle N \rangle / G, M = \#\mathcal{O}(G)$   $\hat{A} = (\hat{a}_{\alpha\beta})_{\alpha,\beta\in\mathcal{O}(G)}, \hat{a}_{\alpha\beta} =: \sum_{j\in\beta} a_{ij}, i \in \alpha, \rho(A) = \rho(\hat{A}), \text{ If } A = A^{T} \text{ then}$   $\hat{A} \text{ symmetric for } \langle \mathbf{x}, \mathbf{y} \rangle = \sum_{\alpha\in\mathcal{O}(G)} (\#\alpha) x_{\alpha} y_{\alpha}.$   $M \geq N/\#G,$ 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  $P_2((v_1, v_2))$ .

#### Graphs of two dimensional pressure for MD

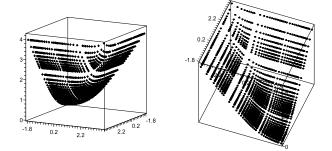


Figure 1: The graph of  $\frac{\bar{P}_1(12,(v_1,v_2))}{12}$  for angles  $\theta = 28^o, \varphi = 78^o$  and  $\theta = -159^o, \varphi = 42^0$ 

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## Graphs of two dimensional density entropy for MD

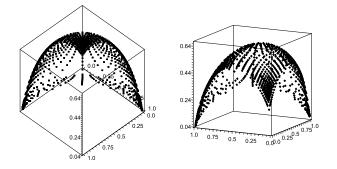


Figure 1: The graph of an approximation of  $\bar{h}_2((p_1, p_2)$  for angles  $\theta = 45^o, \varphi = 45^o$  and  $\theta = -153^o, \varphi = 78^o$ 

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