

# Entropy, pressure, and densities for $\mathbb{Z}^d$ -SOFT

Shmuel Friedland  
University of Illinois at Chicago

Multidimensional symbolic dynamics  
and lattice models of quasicrystals  
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- $\mathbb{Z}$ -SOFT
- Entropies of  $\mathbb{Z}$ -SOFT
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- Entropies of  $\mathbb{Z}^d$ -SOFT
- A symmetricity condition
- Pressure and its conjugate



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 papers and one influential book jointly with Mahadev

**THRESHOLD GRAPHS and related topics**

Uri died September 4, 2009 after a long battle with brain tumor.

View  $[n] = \{1, \dots, n\}$ , as  $n \geq 2$  particles (alphabet)

Hamming distance on  $[n]$ :  $d_h(p, q) = \delta_{pq}$

$\phi : \mathbb{Z} \rightarrow [n]$  configuration  $\phi = \{\phi(i), i \in \mathbb{Z}\}$ ,  $\pi_i(\phi) = \phi(i)$

$[n]^{\mathbb{Z}}$  configurations space, maps from  $\mathbb{Z}$  to  $[n]$

metric on  $[n]^{\mathbb{Z}}$ :  $d(\phi, \psi) = \sum_{i \in \mathbb{Z}} 2^{-|i|} d_h(\phi(i), \psi(i))$

$[n]^{\mathbb{Z}}$ -complete metric space, with diameter 3

The shift map:  $\sigma(\phi)(i) = \phi(i + 1)$ ,  $i \in \mathbb{Z}$

$\mathcal{S} \subset [n]^{\mathbb{Z}}$  subshift:  $\mathcal{S}$ -closed,  $\sigma(\mathcal{S}) = \mathcal{S}$

# $\mathbb{Z}$ -Subshift Of Finite type (SOFT)

$\exists$  finite window  $W \subset \mathbb{Z}$ , admissible configurations  $A \subset [n]^W$

s. t.  $\pi_W(\phi) \in A \iff \phi \in \mathcal{S}$

Near Neighbor SOFT (NNSOFT):  $\exists$  digraph  $\Gamma = ([n], \vec{E})$ :

$\pi_{[2]}(\phi) \in \mathcal{S} \iff (\phi(1), \phi(2)) \in \vec{E}$

Equivalently:  $\phi \in \mathcal{S} \iff (\phi(i), \phi(i+1)) \in \vec{E}$  for all  $i \in \mathbb{Z}, \phi \in \mathcal{S}$

Every NNSOFT is Wang tiling: every dedge  $\vec{pq}$

corresponds to an interval with left and right painted in colors  $p$  and  $q$

Every Wang tiling is NNSOFT: corresponds to a dedge  $\vec{pq}$

NNSOFT is more efficient presentation than Wang tiling for  $\mathbb{Z}$ -SOFT

# Every $\mathbb{Z}$ -SOFT can be coded as NNSOFT

Can assume  $W = [M]$ ,  $M \geq 2$

Code each element of allowable configuration as a particle  $a_1, \dots, a_{|A|}$

view  $a$  and  $b$  as configurations on  $\{1, \dots, M\}$  and  $\{2, \dots, M+1\}$

$\vec{ab}$  allowable iff  $a$  and  $b$  have the same projections on  $\{2, \dots, M\}$

Equivalently  $\pi_{\{2, \dots, M\}}(a) = \pi_{\{1, \dots, M-1\}}(b)$  if  $a, b \in A$ .

$\mathbb{Z}$ -SOFT is a biminfinite walk on a digraph  $\Gamma$

$\Gamma$  symmetric, (undirected graph):  $\vec{pq} \in \Gamma \iff \vec{qp} \in \Gamma$

$\mathbb{Z}$ -SOFT empty set iff  $\Gamma$  has no dicycle

# Entropies of $\mathbb{Z}$ -SOFT I

$W^m(\Gamma)$  -all allowable  $\Gamma$  words of length  $m$ , all walks on  $\Gamma$  of length  $m$

$$|W^{k+m}(\Gamma)| \leq |W^k(\Gamma)| |W^m(\Gamma)| \Rightarrow$$

**subadditivity:**  $\log |W^{k+m}(\Gamma)| \leq \log |W^k(\Gamma)| + \log |W^m(\Gamma)|$

**Fekete lemma:**  $h_{\text{com}}(\mathcal{S}) = \lim_{m \rightarrow \infty} \frac{\log |W^m(\Gamma)|}{m} \leq \frac{\log |W^k(\Gamma)|}{k}, l \in \mathbb{N}$

**Combinatorial entropy, or capacity**

**Theorem:**  $h_{\text{com}}(\Gamma) = h_{\text{top}}(\Gamma)$ -topological entropy of  $\mathcal{S}$

**Proof outline:** Topological entropy is the growth of  $\varepsilon$ -separated points  
equivalent to combinatorial entropy

# Entropies of $\mathbb{Z}$ -SOFT II

$$W^m(\Gamma) = \mathbf{1}^\top A^{m-1} \mathbf{1}, \quad A = A(\Gamma) \text{ adjacency matrix of } \Gamma$$

$$h_{\text{com}}(\Gamma) = \lim_{m \rightarrow \infty} \frac{\log \mathbf{1}^\top A^{m-1} \mathbf{1}}{m} = \log \rho(A)$$

$W_{\text{per}}^m(\Gamma)$ -words of length  $m+1$ : first letter=last letter

$$|W_{\text{per}}^m(\Gamma)| = \text{Tr } A^m, \quad A\mathbf{u} = \rho(A)\mathbf{u}, \quad A^\top \mathbf{v} = \rho(A)\mathbf{v}, \quad \mathbf{v}^\top \mathbf{u} = 1$$

$$h_{\text{per}}(\Gamma) = \limsup_{m \rightarrow \infty} \frac{\log |W_{\text{per}}^m(\Gamma)|}{m} = \log \rho(A)$$

**Theorem:**  $h_{\text{com}}(\Gamma) = h_{\text{top}}(\Gamma) = h_{\text{per}}(\Gamma)$

**Expl.**  $A^m = [a_{ij}^{(m)}] \in \mathbb{Z}_+^{n \times n}$ ,  $a_{ij}^{(m)}$ -#-config:  $\underbrace{i \dots j}_{m+1}$

**A-primitive:**  $A^m = \rho(A)^m \mathbf{u}\mathbf{v}^\top (1 + o(1))$ , else use Frobenius normal form

# The measure of maximal entropy

$C(i_1, \dots, i_m) = \{\phi \in \mathcal{S}, (\phi(1), \dots, \phi(m)) = (i_1, \dots, i_m)\}$ -cylinder of  $\mathcal{S}$

Assume  $\Gamma$  strongly connected  $\iff A = A(\Gamma)$ -irreducible:

$$A = [a_{ij}] \in \{0, 1\}^{n \times n}, \mathbf{A}\mathbf{u} = \rho\mathbf{u}, \mathbf{v}^\top \mathbf{A} = \rho\mathbf{v}^\top, \mathbf{u}, \mathbf{v} > \mathbf{0}, \mathbf{v}^\top \mathbf{u} = 1$$

Measure of maximal entropy, Parry measure:

$$\mu(C(i_1, \dots, i_m)) = \rho(A)^{-m+1} v_{i_1} a_{i_1 i_2} a_{i_2 i_3} \cdots a_{i_{m-1} i_m} u_{i_m}$$

If  $A$  not irreducible,  $\mathcal{S}(\Gamma) \neq \emptyset$  same formulas apply, where  $\mathbf{u}, \mathbf{v} \geq \mathbf{0}$

$\mathbf{u}, \mathbf{v}$  may not be unique:

Frobenius normal (upper triangular) form

# $\mathbb{Z}^d$ -subshift

$[n]^{\mathbb{Z}^d}$ -all configurations  $\phi$  of  $n$ -particles on  $\mathbb{Z}^d$ ,  $d \in \mathbb{N}$

$$d(\phi, \psi) = \sum_{\mathbf{i} \in \mathbb{Z}^d} 2^{-\|\mathbf{i}\|_1} h_d(\phi(\mathbf{i}), \psi(\mathbf{i})).$$

$\pi_X : [n]^{\mathbb{Z}^d} \rightarrow [n]^X$  projection on  $X \subset \mathbb{Z}^d$

$$\mathbf{e}_j = (\delta_{j1}, \dots, \delta_{jd})^\top, j \in [d], \mathbf{1} = (1, \dots, 1)^\top \in \mathbb{Z}^d$$

$j$ -shift:  $\sigma_j(\phi)(\mathbf{i}) = \phi(\mathbf{i} + \mathbf{e}_j), \mathbf{i} \in \mathbb{Z}^d, j \in [d]$

$\mathcal{S} \subset [n]^{\mathbb{Z}^d}$ -subshift, if

$\mathcal{S}$  closed

invariant:  $\sigma_j(\mathcal{S}) = \mathcal{S}, j \in [d]$

$\mathbf{m} = (m_1, \dots, m_d)^\top \in \mathbb{N}^d$ ,  $[\mathbf{m}] = [m_1] \times \dots \times [m_d]$ ,  $\text{vol}(\mathbf{m}) = m_1 \cdots m_d$

$\mathbf{m} + \mathbb{Z}\mathbf{e}_j$ :  $\mathbb{Z}$ -line in direction of axis  $j$  through  $\mathbf{m}$

A subshift  $\mathcal{S} \subset \mathbb{Z}^d$ -is  $\mathbb{Z}^d$ -SOFT:

$\exists$  finite window  $W \subset \mathbb{Z}^d$ , admissible configurations  $A \subset [n]^W$

s. t.  $\pi_W(\phi) \in A \iff \phi \in \mathcal{S}$

# $\mathbb{Z}^d$ -SOFT II

$\mathbb{Z}^d$ -NNSOFT: given by  $\Gamma = (\Gamma_1, \dots, \Gamma_d)$ , digraph  $\Gamma_j = ([n], \vec{E}_j), j \in [d]$

Projection of  $\phi \in \mathcal{S}(\Gamma)$  on  $\mathbf{m} + \mathbb{Z}\mathbf{e}_j$  is  $\mathbb{Z}$ -NNSOFT given by  $\Gamma_j$

$d = 2$ : Every  $\mathbb{Z}^2$ -NNSOFT is Wang tiling

$(\Gamma_1, \Gamma_2)$ -allowable filling of  $[2] \times [2]$  is a Wang tile

square with the colors corresponding di-edges of  $\Gamma_1, \Gamma_2$  respec.

colors of diedges of  $\Gamma_1$  and  $\Gamma_2$  are different

Every Wang tiling is  $\mathbb{Z}^2$ -NNSOFT on  $n$ -number of Wang tiles

$\vec{p}q \in \vec{E}_1$  if tile  $q$  can be to the right of tile  $p$

$\vec{p}q \in \vec{E}_2$  if tile  $q$  can be on top of tile  $p$

# Every $\mathbb{Z}^d$ -SOFT can be coded as NNSOFT

Can assume  $W = [\mathbf{M}]$ ,  $\mathbf{M} = (M_1, \dots, M_d) \geq 2 \cdot \mathbf{1}$

Code each element of allowable configuration as a particle  $a_1, \dots, a_{|A|}$

Assume  $a$  and  $b$  allowable configurations on  $[\mathbf{M}]$

$\vec{ab} \in \vec{E}_1$  if

$\pi_{\{2, \dots, M_1\} \times [M_2] \times \dots \times [M_d]}(a) = \pi_{\{1, \dots, M_1-1\} \times [M_2] \times \dots \times [M_d]}(b)$  if  $a, b \in A$

similar conditions for  $\vec{ab} \in \vec{E}_j, j > 1$

$d = 2$ :  $\vec{ab} \in \vec{E}_2$  if

$\pi_{[M_1] \times \{2, \dots, M_2\}}(a) = \pi_{[M_1] \times \{1, \dots, M_2-1\}}(b)$  if  $a, b \in A$

# Decidability of $\mathbb{Z}^2$ -SOFT

**Köning 1927**  $\Rightarrow \mathbb{Z}^2$ -NNSOFT nonempty iff  $W^{(n,n)}(\Gamma) \neq \emptyset \quad \forall n \in \mathbb{N}$

**Outline of proof:**  $T_k = [-2^k, 2^k]^2 \cap \mathbb{Z}^2, k \in \mathbb{N}$ ,  $\Theta_k$ -admissible

configuration of  $T_k$ . Choose infinite subseq.  $\{\Theta_{k_i^1}\}_{i=1}^\infty$  with same

projection on  $T_1$ . Choose infinite subsequence  $\{\Theta_{k_i^2}\}_{i=1}^\infty$  of  $\{\Theta_{k_i^1}\}_{i=1}^\infty$

same projection on  $T_2$ , and so on. Take Cantor diagonal subsequence.

**Wang:**  $\mathcal{S}(\Gamma)$ -decidable if either  $\exists$  periodic configuration or  $\mathcal{S}(\Gamma) = \emptyset$

**Berger 1966:**  $\exists$  nondecidable Wang tiling = nonperiodic (Gamard lec.)

**Shahar Mozes 1989:**  $\mathbb{Z}^2$ -ergodic theory yields nonperiodic Wang tilings

**Jeandel-Rao 2021:** 11 Wang tiles with 4 colors -minimal example

# Combinatorial entropy of $\mathbb{Z}^d$ -SOFT I

$$\mathbf{m} = (m_1, \dots, m_d) \in \mathbb{N}^d, d > 1, p \in [d],$$

$$\mathbf{m}^{\hat{p}} = (m_1, \dots, m_{p-1}, m_{p+1}, \dots, m_d), \mathbf{m} = (\mathbf{m}^{\hat{p}}, m_p)$$

$W^{\mathbf{m}}(\Gamma)$  -allowable  $\Gamma$  configuration on box  $[\mathbf{m}]$

$$|W^{(\mathbf{m}^{\hat{p}}, j+k)}(\Gamma)| \leq |W^{(\mathbf{m}^{\hat{p}}, j)}(\Gamma)| |W^{(\mathbf{m}^{\hat{p}}, k)}(\Gamma)| \Rightarrow$$

**$p$ -subadditivity:**  $\log |W^{(\mathbf{m}^{\hat{p}}, j+k)}(\Gamma)| \leq \log |W^{(\mathbf{m}^{\hat{p}}, j)}(\Gamma)| + \log |W^{(\mathbf{m}^{\hat{p}}, k)}(\Gamma)|$

$$(1) \log \rho(p, \mathbf{m}^{\hat{p}}) := \lim_{j \rightarrow \infty} \frac{\log |W^{(\mathbf{m}^{\hat{p}}, j)}(\Gamma)|}{j} \leq \frac{\log |W^{(\mathbf{m}^{\hat{p}}, j)}(\Gamma)|}{j}$$

$\rho(p, \mathbf{m}^{\hat{p}})$ -spectral radius  $\mathbb{Z}$ -NNSOFT in direction  $p$  on states  $W^{\mathbf{m}^{\hat{p}}}(\Gamma^{\hat{p}})$

# Combinatorial entropy of $\mathbb{Z}^d$ -SOFT II

Fix  $j$ , observe  $\frac{\log |W^{(\mathbf{m}^{\hat{\rho}}, j)}(\Gamma)|}{j}$  subadditive in variable  $q \in [d] \setminus \{p\}$

$\log \rho(p, \mathbf{m}^{\hat{\rho}})$ -subadditive in each variable in  $[d] \setminus \{j\}$

$$(2) h_{com}(\Gamma) = \lim_{\mathbf{m} \rightarrow \infty} \frac{\log |W^{\mathbf{m}}(\Gamma)|}{\text{vol}(\mathbf{m})} \leq \frac{\log \rho(p, \mathbf{m}^{\hat{\rho}})}{\text{vol}(\mathbf{m}^{\hat{\rho}})} \leq \frac{\log |W^{\mathbf{m}}(\Gamma)|}{\text{vol}(\mathbf{m})}, \mathbf{k} \in \mathbb{N}^d$$

$$\log 0 = -\infty \Rightarrow h_{com}(\Gamma) \in \{-\infty\} \cup \mathbb{R}_+$$

**Theorem:**  $h_{com}(\Gamma) = h_{top}(\Gamma)$ -topological entropy of  $\mathcal{S}(\Gamma)$

# No periodic solution for nonempty $\mathbb{Z}^d$ -NNSOFT

**periodic state:**  $\phi \in \mathcal{S}_{per,m}(\Gamma)$ ,  $\phi(\mathbf{i} + m_j \mathbf{e}_j) = \phi(\mathbf{i})$ ,  $\mathbf{i} \in \mathbb{Z}^d$ ,  $m_j \in \mathbb{N}$ ,  $j \in [d]$

$$W_{per}^m(\Gamma) = \{\pi_{[m+1]}(\phi), \phi \in \mathcal{S}_{per,m}(\Gamma)\}$$

all states in  $W^m(\Gamma)$  extending to periodic states in  $\mathcal{S}_{per,m}(\Gamma)$

**Lemma:** Assume  $d > 1$ ,  $p \in [d]$  and  $W^{m\hat{p}}(\Gamma^{\hat{p}})$  nonempty.

$\mathcal{S}_{(m\hat{p})}(\Gamma) = \emptyset$ , iff  $\mathbb{Z}$ -SOFT induced by  $\Gamma_p$  on  $W^{m\hat{p}}(\Gamma^{\hat{p}})$  is empty

equivalently  $A^{W^{m\hat{p}}|_{(\Gamma^{\hat{p}})}(\rho, W^{m\hat{p}}(\Gamma^{\hat{p}})) = 0$

**Corollary**  $\mathcal{S}((\Gamma_1, \Gamma_2))$  has no periodic states iff for each  $i \in \mathbb{N}$  s.t.

$W_{per}^i(\Gamma_1) \neq \emptyset$ ,  $\mathbb{Z}$ -SOFT induced by  $\Gamma_2$  on  $W_{per}^i(\Gamma_1)$  is empty

# Periodic entropies

$$\log 0 = -\infty$$

$$h_{per}(\Gamma) = \limsup_{\mathbf{m} \rightarrow \infty} \frac{\log |W_{prod}^{\mathbf{m}}(\Gamma)|}{vol(\mathbf{m})} \in \{-\infty\} \cup \mathbb{R}_+$$

**Theorem (Friedland 1997)** If  $d - 1$  digraphs in  $(\Gamma_1, \dots, \Gamma_d)$  are symmetric then  $h_{top}(\Gamma) = h_{per}(\Gamma)$ , and the entropy is computable

# The case $d = 2$ and $\Gamma_1$ symmetric I

**Claim:**  $\mathcal{S}(\Gamma) \neq \emptyset \iff \rho(2, 2) > 0$

**Proof:**  $\rho(2, 2) > 0 \iff W^{(2,i)}(\Gamma) \neq \emptyset \forall i \geq 2$

**Assume**  $W^{(2,i)}(\Gamma) \neq \emptyset$ ,  $A(1, i) \in \{0, 1\}^{N \times N}$ ,  $N = |W^i(\Gamma_2)|$

**nonzero symmetric transfer matrix on states in  $W^i(\Gamma_2) \Rightarrow$**

$W^{i,i}(\Gamma) \neq \emptyset \Rightarrow \mathcal{S}(\Gamma) \neq \emptyset$

# The case $d = 2$ and $\Gamma_1$ symmetric II

$W_{per,1}^{(k,i)}(\Gamma)$ - $i$ -states induced by  $\Gamma_2$  on  $W_{per}^k(\Gamma_1)$

$A_{per}(2, k)$ -transfer matrix in direction 2 on states  $W_{per}^k(\Gamma_1)$

Observe  $\rho_{per}(2, k) = \rho(A_{per}(2, k)) \leq \rho(2, k)$  (explained later)

$A(1, i)^{2m} \succeq 0 \Rightarrow \rho(1, i)^{2m} = \rho(A^{2m}(1, i)) \leq \text{Tr } A^{2m}(1, i) =$

$|W_{per,1}^{(2m,i)}(\Gamma)| = \mathbf{1}^\top A_{per}^{i-1}(2, 2m)\mathbf{1}, \mathbf{1} \in \mathbb{R}^N, N = |W_{per}^{2m}(\Gamma_1)|$

$\frac{\log \rho(1, i)}{i} \leq \frac{\log |W_{per,1}^{(2m,i)}(\Gamma)|}{(2m)i} = \frac{\log |W_{per}^{(2m,i)}(\Gamma)|}{(2m)i}$  for  $i \gg 1$  fixed  $m$

$i \rightarrow \infty \Rightarrow \frac{\log \rho(1, i)}{i} = h(\Gamma) \leq \frac{\log \rho_{per}(2, 2m)}{2m}$  (3)

let  $m \rightarrow \infty \Rightarrow h_{com}(\Gamma) \leq h_{per}(\Gamma) \Rightarrow h_{com}(\Gamma) = h_{per}(\Gamma)$

# Computability of $h(\Gamma)$ for $d = 2$ and $\Gamma_1$ symmetric

$$(4) \frac{\log \rho(1, p+2q+1)}{p} - \frac{\log \rho(1, 2q+1)}{p} \leq h(\Gamma) \leq \frac{\log \rho_{per}(2, 2m)}{2m}, p \in \mathbb{N}, q \in \mathbb{Z}_+$$

RHS of (5) is shown in (3)

max characterization of  $\rho(1, i)^p \geq \frac{\mathbf{x}^\top A(1, i)^p \mathbf{x}}{\mathbf{x}^\top \mathbf{x}}$  choose  $\mathbf{x} = A(1, i)^q \mathbf{1} \Rightarrow$

$$\frac{\log \rho(1, i)}{i} \geq \frac{\log \mathbf{1}^\top A(1, i)^{p+2q} \mathbf{1}}{pi} - \frac{\log \mathbf{1}^\top A(1, i)^{2q} \mathbf{1}}{pi} = \frac{\log W^{\rho+2q+1, i}(\Gamma)}{pi} - \frac{\log W^{2q+1, i}(\Gamma)}{pi}$$

let  $i \rightarrow \infty$  to obtain LHS of (4)

$$\text{Use (2) and } q = 0: \frac{\log \rho(1, p+1)}{p} - \frac{\log \rho(1, 1)}{p} \leq h(\Gamma) \leq \frac{\log \rho(1, p+1)}{p+1} \quad (5)$$

Markley-Paul 1981 showed (5) for primitive symmetric  $A(\Gamma_1)$

Note that computation of  $\rho(1, p+1)$  is exponential in  $p$

as the number of nonzero entries of  $A(1, p+1)$  is at least  $O(\rho(2, 2)^{p+1})$

# Observations on $\rho_{per}(j, q)$ and $\rho(j, q)$

Assume  $\mathcal{S}((\Gamma_1, \Gamma_2)) \neq \emptyset$

Claim  $\rho_{per}(j, q) \leq \rho(j, q)$  for  $j \in [2], q \geq 2, \rho(2, q) \leq \rho(2, q + 1)$

Proof: Enough to assume  $\rho_{per}(2, q) \geq 1$ . View

$A_{per}(2, q) = [a_{st}], s, t \in W^q(\Gamma_1)$  s.t.  $a_{st} = 0$ , unless  $s, t \in W_{per}^q(\Gamma_1)$

$A_{per}(2, q) \leq A(2, q) \Rightarrow \rho_{per}(2, q) \leq \rho(2, q)$

As  $\Gamma_1$  symmetric extend each  $k$ -walk to  $k + 1$  walk by reversing

last edge  $\Rightarrow A(2, k)$  prin. subm. of  $A(2, k + 1) \Rightarrow \rho(2, k) \leq \rho(2, k + 1)$

$\Gamma_1$  symmetric  $\Rightarrow \lim_{k \rightarrow \infty} \frac{\log \rho(2, k)}{k} = \limsup_{k \rightarrow \infty} \frac{\log \rho_{per}(2, k)}{k} = h(\Gamma)$

# Residual entropy of ice

$\mathbb{Z}^2$ -NNSOFT particles, where no two same particles are adjacent

$\Gamma_1 = \Gamma_2 = K_3$ -complete graph on 3 vertices (symmetric)

E. Lieb computed periodic entropy 1967:

$$h(\Gamma) = \frac{3}{2} \log \frac{4}{3} = \log (4/3)^{3/2} = 0.43152 \dots$$

$h(\Gamma)$  not a log of algebraic integer as for  $\mathbb{Z}$ -SOFT

For  $p = 2$  lower bound in (5) is 0.4122579570

Upper bound in (4) for  $m = 2$ : 0.462989385

# Monomer-dimer model in $\mathbb{Z}^d$

A monomer is a particle that occupies a point in  $\mathbb{Z}^d$ ,

or a  $d$ -unit cube centered at a point in  $\mathbb{Z}^d$

A dimer is a domino in positioned in direction  $\mathbf{e}_j, j \in \mathbb{Z}^d, j \in [d]$

or two glued unit cubes

One can consider just dimers without monomers

The dimer coding correspond to  $n = 2d$  particles

The monomer-dimer model corresponds to  $n = 2d + 1$  particles

$\mathbb{Z}^2$ -dimer entropy is  $\frac{1}{\pi} = \sum_{i=0}^{\infty} \frac{(-1)^i}{(2i+1)^2} = 0.29156090\dots$

# Density of the Monomer-dimer model

For a fixed  $p \in [0, 1]$ :  $W_{p_1, p_2}^m(\Gamma) \subset W^m(\Gamma)$ -all configurations with density of dimers  $\in (p_1, p_2)$

$$h((p_1, p_2), \Gamma) = \lim_{m \rightarrow \infty} \frac{\log |W_{p_1, p_2}^m(\Gamma)|}{|W^m(\Gamma)|}, \quad h(p, \Gamma) = \lim_{p_1 \rightarrow p} h((p_1, p), \Gamma)$$

**Claim**  $h(\Gamma) = \max_{p \in [0, 1]} h(p, \Gamma)$

# Pressure function for an external field

$c_i(\phi)$ -#  $i$ -particles in  $\phi \in W^{\mathbf{m}}(\Gamma)$ ,  $\mathbf{c}(\phi) = (c_1(\phi), \dots, c_n(\phi))^{\top} \in \mathbb{Z}_+^n$

$W^{\mathbf{m}}(\Gamma, \mathbf{c}) = \{\phi \in W^{\mathbf{m}}(\Gamma), \mathbf{c}(\phi) = \mathbf{c}\}$ ,  $\mathbf{c} \in \text{vol}(\mathbf{m})\Pi_n \cap \mathbb{Z}_+^n$

$P_{\Gamma}(\mathbf{u}, \mathbf{m}) = \frac{\log \sum_{\phi \in W^{\mathbf{m}}(\Gamma)} \exp(\mathbf{c}(\phi)^{\top} \mathbf{u})}{\text{vol}(\mathbf{m})}$ ,  $\mathbf{u} = (u_1, \dots, u_n)^{\top} \in \mathbb{R}^n$

$P_{\Gamma}(\mathbf{u}, \mathbf{m})$ -convex in  $\mathbf{u}$ , subadditive in each  $m_i$

$\nabla P_{\Gamma}(\mathbf{u}, \mathbf{m}) \in \mathbb{P}_n$  - the set of probability vectors in  $\mathbb{R}^n \Rightarrow$

$|P_{\Gamma}(\mathbf{v}, \mathbf{m}) - P_{\Gamma}(\mathbf{u}, \mathbf{m})| \leq \|\mathbf{v} - \mathbf{u}\|_{\infty}$

$P_{\Gamma}(\mathbf{u} + t\mathbf{1}, \mathbf{m}) = t + P_{\Gamma}(\mathbf{u}, \mathbf{m}) \Rightarrow$  can assume  $u_n = 0$

$P_{\Gamma}(\mathbf{u}) := \lim_{\mathbf{m} \rightarrow \infty} P_{\Gamma}(\mathbf{u}, \mathbf{m}) \leq P_{\Gamma}(\mathbf{u}, \mathbf{m})$

convex,  $|P_{\Gamma}(\mathbf{v}) - P_{\Gamma}(\mathbf{u})| \leq \|\mathbf{v} - \mathbf{u}\|_{\infty}$

subgradient  $\partial P_{\Gamma}(\mathbf{u}) \in \Pi_n$  exists  $\forall \mathbf{u} \in \mathbb{R}^n$ ,  $\nabla P_{\Gamma}(\mathbf{u}) \exists$  a.e.

# Pressure function for an external field for $\mathbb{Z}$ -SOFT

$$d = 1: P_{\Gamma}(\mathbf{u}) = \log \rho(A(\Gamma, \mathbf{u})), \quad A(\Gamma, \mathbf{u}) = [a_{ij} \exp((u_i + u_j))/2]$$

$A(\Gamma)$ -irreducible  $\Rightarrow P_{\Gamma}(\mathbf{u})$  analytic in  $\mathbf{u}$ , and

$\Pi_{\Gamma}$ -a convex hull of probability vectors

corresponding to uniform distribution on cycles in  $\Gamma$

**Example:**  $\Gamma$  has one cycle on  $[n]$ :  $\Pi_{\Gamma} = \{\frac{1}{n}\mathbf{1}\}$

$$P_{\Gamma}(\mathbf{u}) = \frac{\sum_{i=1}^n u_i}{n}, \quad \nabla P_{\Gamma}(\mathbf{u}) = \frac{1}{n}\mathbf{1} \quad \forall \mathbf{u} \in \mathbb{R}^n$$

$A(\Gamma)$  reducible- $\Gamma$  has  $k$ -strongly connected components  $\Gamma_1, \dots, \Gamma_j$

$$P_{\Gamma}(\mathbf{u}) = \max_{j \in [k]} \log A(\Gamma_j, \mathbf{u}_j)$$

It is possible that  $P_{\Gamma}(\mathbf{u})$ -not differentiable at some points

# Density points

$\mathbf{p} \in \Pi_n$  is a **density point of**  $\mathcal{C}(\mathbb{Z}^d)$ :  $\exists \{\mathbf{m}_q\} \subset \mathbb{N}^d, \mathbf{c}_q \in (\text{vol}(\mathbf{m}_q)\Pi_n) \cap \mathbb{Z}_+^n,$

$$W^{\mathbf{m}_q}(\Gamma, \mathbf{c}_q) \neq \emptyset, q \in \mathbb{N}, \quad (5) \quad \lim_{\mathbf{m}_q \rightarrow \infty} \frac{1}{\text{vol}(\mathbf{m}_q)} \mathbf{c}_q = \mathbf{p} (\in \Pi_n)$$

$\Pi_\Gamma$  **closed nonempty set of density pts** (Cantor diagonal sequence)

$$h_\Gamma(\mathbf{p}) = \limsup_{\mathbf{m}_q \rightarrow \infty} \frac{\log |W^{\mathbf{m}_q}(\Gamma, \mathbf{c}_q)|}{\text{vol}(\mathbf{m}_q)} (\geq 0) \text{ for all } \mathbf{m}_q \text{ satisfying (5)}$$

$h_\Gamma(\mathbf{p})$  - **density entropy**

is **upper-semicontinuous on**  $\Pi_\Gamma$

# Conjugate pressure function I

**Legendre-Fenchel transform:**  $P_\Gamma^*(\mathbf{v}) := \sup_{\mathbf{u} \in \mathbb{R}^n} \mathbf{v}^\top \mathbf{u} - P_\Gamma(\mathbf{u}), \mathbf{v} \in \mathbb{R}^m$

**convex,**  $\mathbf{v} \in \partial P_\Gamma(\mathbf{u}) \Rightarrow P_\Gamma^*(\mathbf{v}) = \mathbf{v}^\top \mathbf{u} - P_\Gamma(\mathbf{u})$

$\{\mathbf{v}, P_\Gamma^*(\mathbf{v}) < \infty\} = \text{dom } P_\Gamma^* \supseteq \partial P_\Gamma(\mathbb{R}^n) \supseteq \text{r.i. dom}(P_\Gamma^*), \quad P_\Gamma^{**} = P_\Gamma$

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$h_\Gamma(\mathbf{p}) \leq -P_\Gamma^*(\mathbf{p}), \quad \mathbf{p} \in \Pi_\Gamma, \quad \text{dom } P_\Gamma^* = \text{conv } \Pi_\Gamma$

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

$P_\Gamma(\mathbf{0}) = h_\Gamma = \max_{\mathbf{p} \in \Pi_\Gamma} h_\Gamma(\mathbf{p})$

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

$h_\Gamma(\mathbf{p}) = P_\Gamma(\mathbf{u}) - \mathbf{p}^\top \mathbf{u} = -P_\Gamma^*(\mathbf{p})$  for  $\mathbf{p} \in \Pi_\Gamma(\mathbf{u}), \mathbf{u} \in \mathbb{R}^n$

# Conjugate pressure function II

Generalization of Hammersley for the monomer-dimer entropy:

$h_\Gamma$  is concave on a convex subset of  $\Pi_\Gamma$

$h_\Gamma(\mathbf{p}) = -P_\Gamma^*(\mathbf{p})$  continuous, has subdifferential on

$$\Pi_\Gamma(\mathbb{R}^n) = \cup_{\mathbf{u} \in \mathbb{R}^n} \Pi_\Gamma(\mathbf{u}),$$

If  $[n]$  has a friendly particle, or configuration then  $\Pi_\Gamma$  is convex

For monomer-dimer  $\mathbb{Z}^d$ -SOFT, full  $d$ -dimers and monomer  
are friendly configurations

# Identification of particles

In the study of monomer-dimer models one identifies dimers in each direction  $i \in [d]$  in pressure function

Computation of pressure function reduces to a function in one variable

In general  $\mathbb{Z}^d$ -SOFT identify  $i \equiv j$  by letting  $u_i = u_j$  in  $P_\Gamma(\mathbf{u})$

# First order phase transition

First order phase transition (FOPT) at  $\mathbf{u} \in \mathbb{R}^n$  if  $\nabla P_\Gamma(\mathbf{u})$ -does not exist

$$h_\Gamma = 0 \Rightarrow P_\Gamma = \max_{\mathbf{p} \in \Pi_\Gamma} \mathbf{p}^\top \mathbf{u} = \max_{\mathbf{p} \in \text{conv } \Pi_\Gamma} \mathbf{p}^\top \mathbf{u}$$

In this case FOPT for  $\mathbf{u} \neq \mathbf{0}$  if supporting hyperplane to  $\text{conv } \Pi_\Gamma$

orthogonal to  $\mathbf{u}$  passes at least through two points in  $\Pi_\Gamma$

# Hammersley's results

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  $[0, 1]$   
Heilmann and Lieb 72:  $h_d(p)$  analytic on  $(0, 1)$   
No phase transition in parameter  $p \in (0, 1)$

# Graph estimates for $h_2(p)$

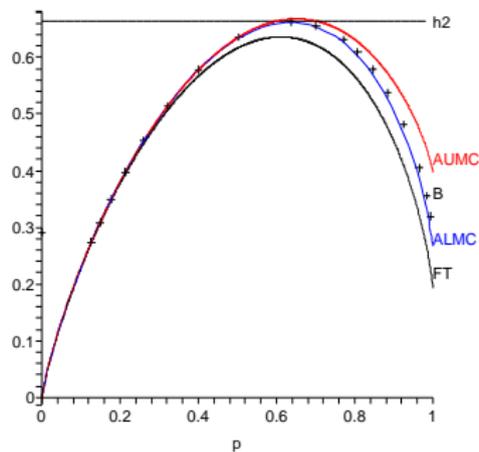


Figure 1: Monomer-dimer tiling of the 2-dimensional grid: entropy as a function of dimer density. FT is the Friedland-Tverberg lower bound,  $h_2$  is the true monomer-dimer entropy. B are Baxter's computed values. ALMC is the Asymptotic Lower Matching Conjecture. AUMC is the entropy of a countable union of  $K_{4,4}$ , conjectured to be an upper bound by the Asymptotic Upper Matching Conjecture.

# Graphs of two dimensional pressure for MD

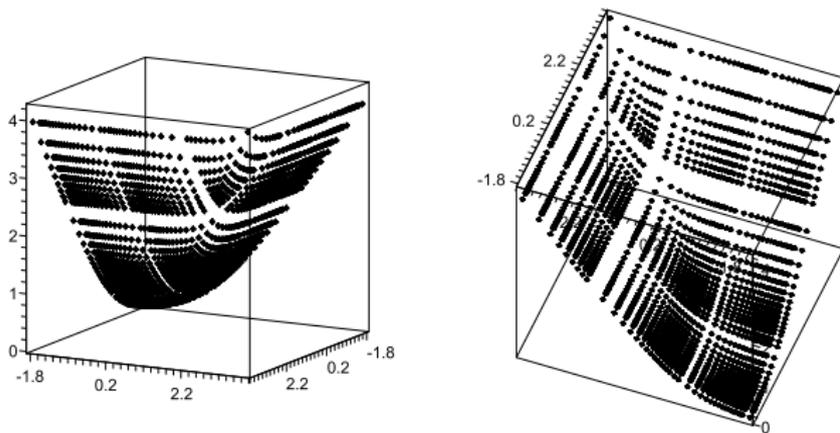


Figure 1: The graph of  $\frac{\bar{P}_1(12, (v_1, v_2))}{12}$  for angles  $\theta = 28^\circ, \varphi = 78^\circ$  and  $\theta = -159^\circ, \varphi = 42^\circ$

# Graphs of two dimensional density entropy for MD

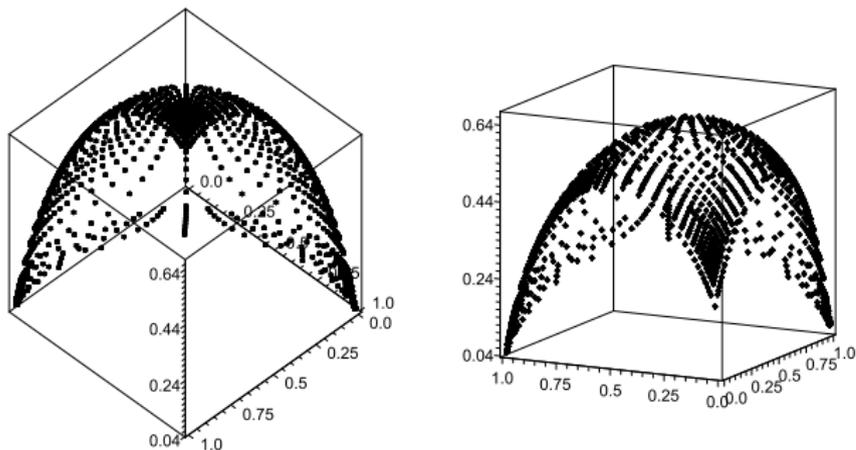


Figure 1: The graph of an approximation of  $\bar{h}_2((p_1, p_2))$  for angles  $\theta = 45^\circ, \varphi = 45^\circ$  and  $\theta = -153^\circ, \varphi = 78^\circ$

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