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EXACTLY SOLVABLE MEAN-FIELD MONOMER-DIMER MODELS

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- Monomer-Dimer models describe systems with hard-core interactions.

- Physical origins: bi-atomic oxygen molecules deposited on tungsten (and other phenomena).

- Early rigorous results: Kasteleyn, Fisher and Temperley (pure dimer case, 60ies) and <u>especially</u> Heilmann and Lieb (70ies) on the absence of phase transitions.

- ... up to recent results.

- In computer science: properties of size and number *matching*. This is related to the entropy of the MD model. Problem is studied for random graphs and also in presence of attractive interaction among dimers.

- in physics: the attractive component of the Van der Waals potential.

Definitions

- $G = (V, E)$ graph with vertex set V and edge set $E \subseteq \{uv \equiv \{u, v\} \,|\, u, v \in V,\, u \neq v\}$.

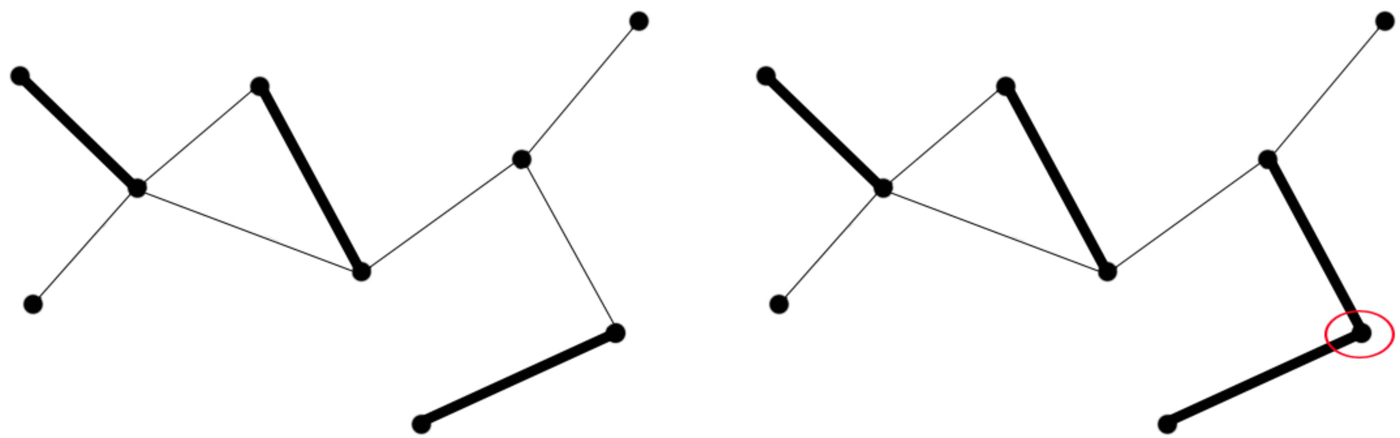
- A *Dimeric Configuration* D on the graph G is a family of edges with no vertex in common.

- We associate to it the *monomeric configuration*:

$$\mathscr{M}_G(D) := \{v \in V \,|\, \forall u \in V \; uv \notin D\}\,.$$

- Notice that hard-core interaction imposes the constraint

$$2\,|D| + |\mathscr{M}_G(D)| = |V|$$



Allowed (left) and forbidden (right) dimeric configuration.

A monomer-dimer model on G is defined by assigning activites to monomers and dimers, $x > 0$, $w > 0$, and considering the measure

$$\mu_{G,x,w}(D) = \frac{1}{Z_G(x,w)} x^{|\mathscr{M}_G(D)|} w^{|D|} \ .$$

The constraint between vertices, monomers and dimers implies

$$Z_G(x,w) \ = \ w^{|V|/2} \, Z_G\Big(\frac{x}{\sqrt{w}}\,, 1\Big) \, .$$

Without loss of generality we assume $w = 1$ and study

$$\mu_{G,x}(D) = \frac{1}{Z_G(x)} \, x^{|V|-2\,|D|} \quad \forall D \in \mathscr{D}_G \, ,$$

and the pressure

$$P_G(x) = \ln Z_G(x)$$

Among the main quantities of interest the *monomer density* is defined as

$$\varepsilon_G(x) := x \frac{\partial}{\partial x} \frac{P_G(x)}{|V|} = \Big\langle \frac{|\mathscr{M}_G|}{|V|} \Big\rangle_{G,x} \,,$$

it also useful to consider the probability of having a monomer on a given vertex $o \in V$:

$$\mathcal{R}_x(G,o) := \langle \mathbb{1}_{o \in \mathscr{M}_G} \rangle_{G,x} \in [0,1] \,,$$

whose relation with the monomer density is

$$\varepsilon_G(x) = \frac{1}{|V|} \sum_{o \in V} \mathcal{R}_x(G,o) \,.$$

Basic property. Defining:

- $u \sim v$ two *neighbours* in the graph G,

- E_o the set of edges which connect the vertex $o \in V$ to one of its neighbours,

- $G - o := (V \setminus o, E \setminus E_o)$

the Heilmann-Lieb identity holds:

$$Z_G(x) = x\, Z_{G-o}(x) + \sum_{v \sim o} Z_{G-o-v}(x)\,.$$

The identity can be used to solve any finite graph, and some limiting cases:

- the line: the partition function for N sites is the N-th Chebyshev polynomial of the second type.

- the ρ-regular rooted tree (line is ρ=1): the partition function for K generations is a product of all the k-th, $1 \leq k \leq K$, Chebyshev polynomial of the second type.

- the complete graph, related to the Hermite polynomials (suitably rescaled with $\sqrt{N}$ for the dimer contribution).

Plan of the talk. Report on two results, two exact solutions:

- Mean-field (complete graph) with attractive potential among similar particles.

- Mean-field (quenched measure) on a class of diluted graphs (locally tree-like).

- ...

1) Exact Solution for the Attractive Case

Diego Alberici, P.C., Emanuele Mingione:
JMP 2014, EPL 2014

Configurations with two nearest-neighbor monomers (or dimers) are favoured:

$$\mu_{N,(h,J)}(D) = \frac{1}{Z_N(h,J)}\, e^{(h+1/2\ln N)|\mathscr{M}_N(D)|+J/N|\mathscr{N}_N(D)|}$$

$\mathscr{N}_N(D)$ is the set of neighbouring monomers and $J > 0$.

Results:

$$\exists \quad p = \lim_{N\to\infty} \frac{1}{N} \ln Z_N \ ,$$

$$p = \sup_{m\in[0,1]} \tilde{p}(m) \ ,$$

$$\tilde{p}(m) \ = \ -\frac{J}{2} m^2 + p^{\mathrm{MD}}(J\, m + h) \ .$$

p^{MD} is the pure ($J = 0$) monomer-dimer pressure in the complete graph

$$p^{\mathrm{MD}}(\xi) = -\frac{1}{2}(1 - g(\xi)) - \frac{1}{2}\ln(1 - g(\xi))$$

where $g(\xi) = \frac{1}{2}(\sqrt{e^{4\xi} + 4e^{2\xi}} - e^{2\xi})$.

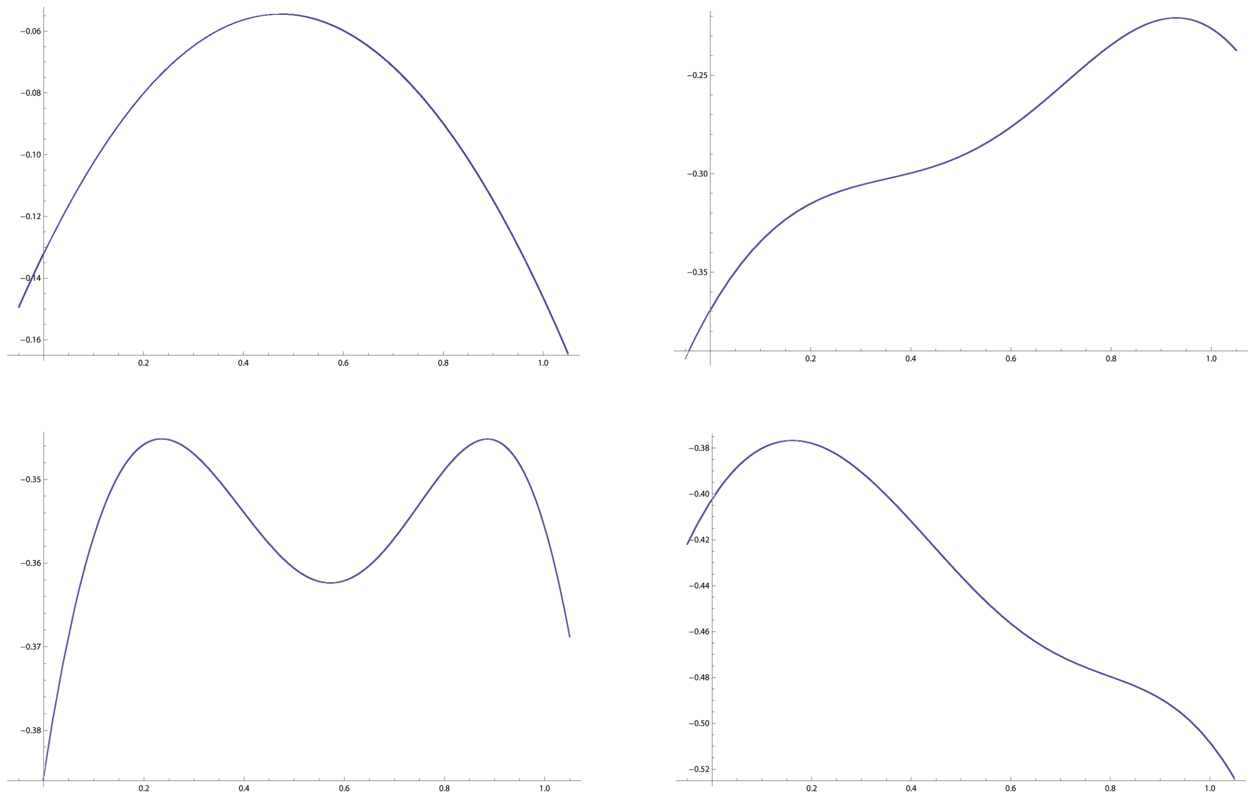
The stationarity condition for $\tilde{p}$ gives:

$$m \, = \, g(J\, m + h) \; ,$$

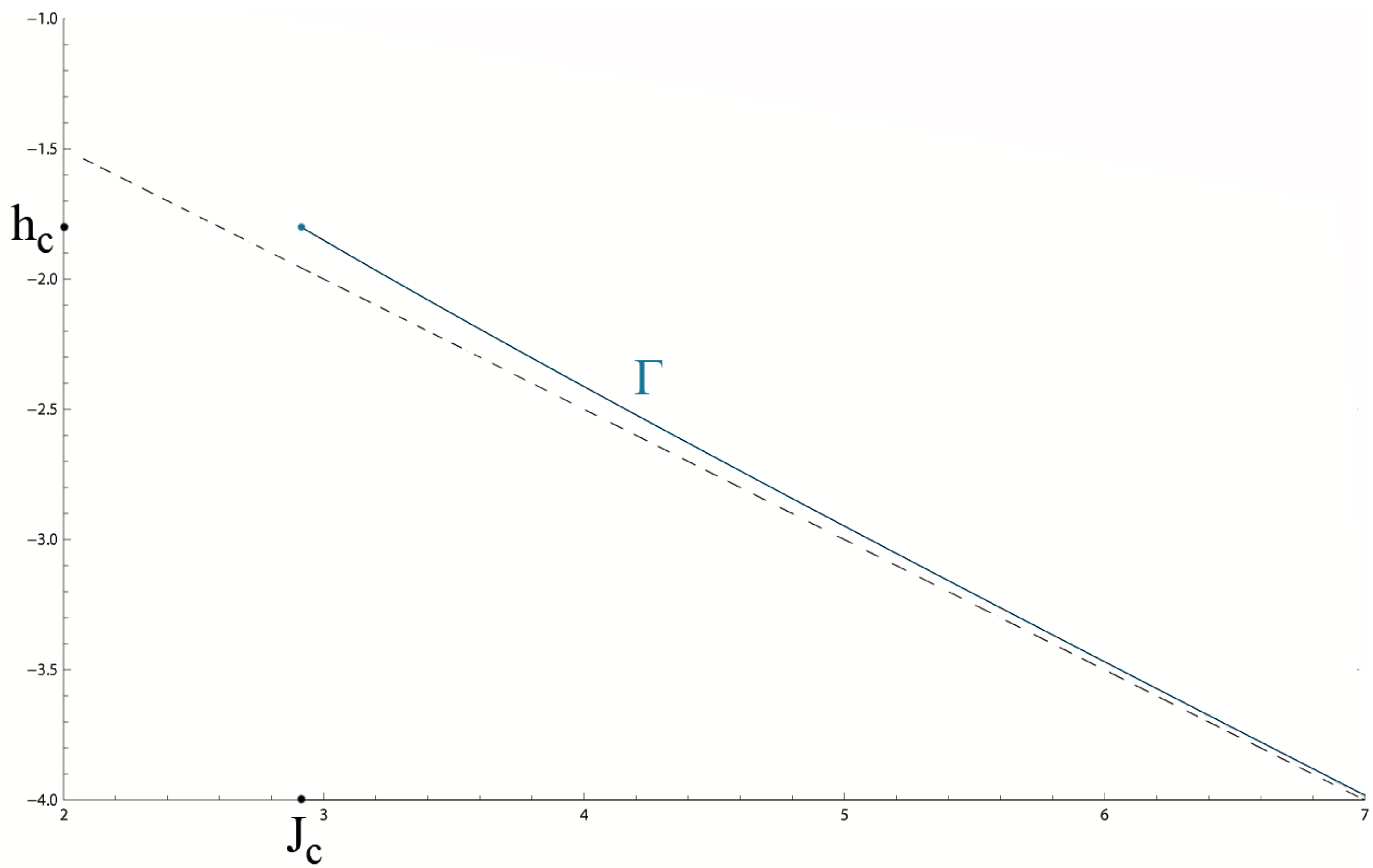
with critical point

$$\Big(J_c,\, h_c\Big) \, = \, \Big(\tfrac{3+2\,\sqrt{2}}{2},\, \tfrac{1}{2}\ln(2\,\sqrt{2} - 2) - \tfrac{2+\sqrt{2}}{2}\Big) \; ,$$

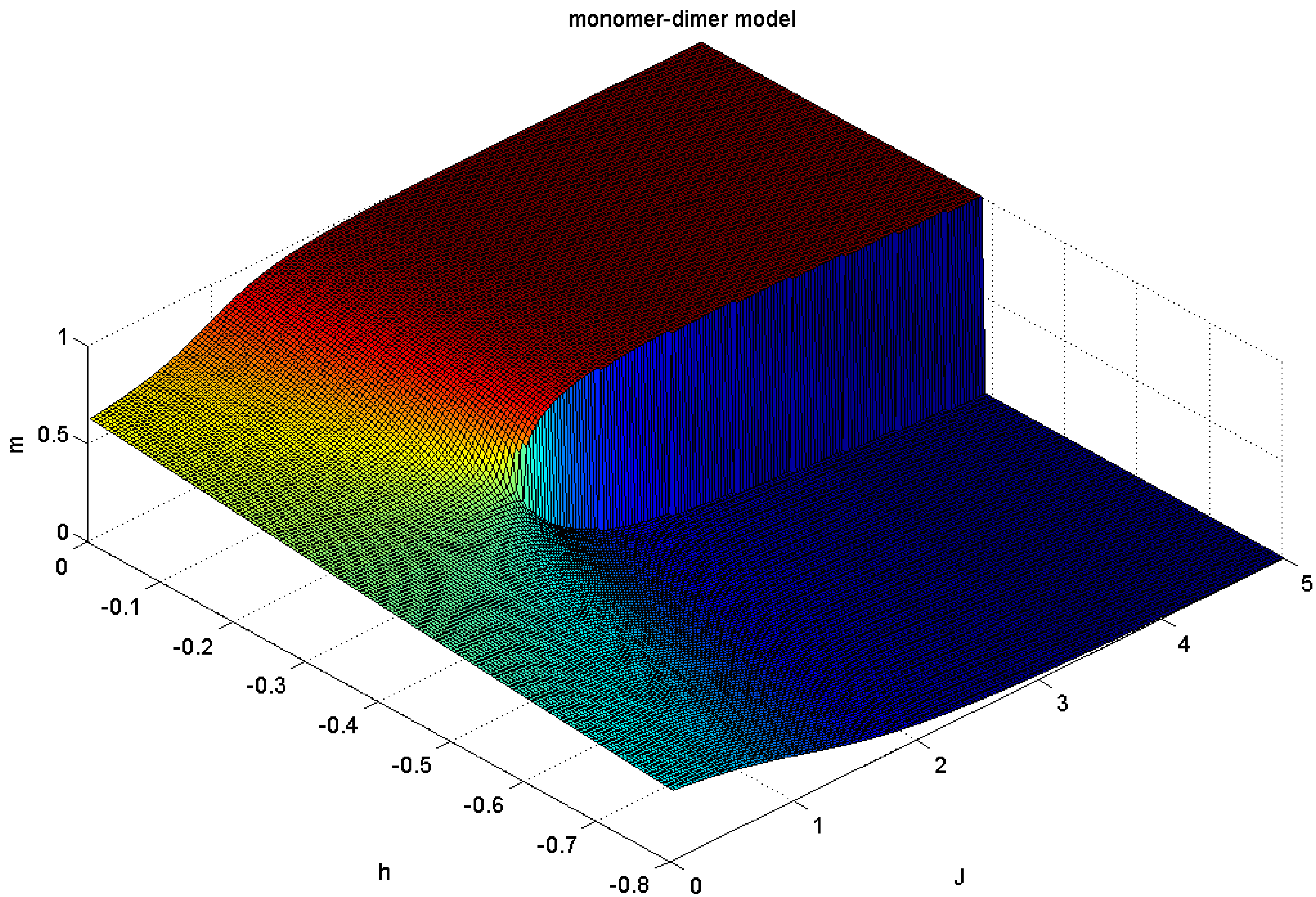
critical exponents 1/2 and 1/3, a coexistence curve Γ in the (J,h) plane with first order phase transition.



The function $\tilde{p}$ plotted versus m, for different values of the parameters J and h.



The critical curve, its asymptote and the critical point (Jc, hc) represented on the half plane (J, h).



The coexistence surface with the transition.

Proof Ideas

- new variational principle, upper and lower bounds

Theorem:

$$p_N \geq -\frac{J}{2} m^2 + p^{\mathsf{MD}}(J\, m + h - \frac{J}{2N})$$

$$p_N \leq \frac{\ln(N+1)}{N} + \sup_m \{-\frac{J}{2} m^2 + p^{\mathsf{MD}}(J\, m + h - \frac{J}{2N})\}$$

2) Exact Solution for the Diluted Case

Diego Alberici, P.C.:
CMP 2014

Dilution is introduced through a *random graph* structure of Erdös-Rényi type: each vertex has a Poisson(c) distributed number of neighbors.

This graph is *locally tree-like* and all the results were proved for sequences of random graphs $(G_n)_{n\in\mathbb{N}}$ locally convergent to a unimodular Galton-Watson tree $\mathcal{T}(P,\rho)$ and with finite second moment of the asymptotic degree distribution P.

Results

Consider the random variable $Y(x)$ whose distribution is defined as the only fixed point supported in $[0,1]$ of the distributional equation

$$Y \stackrel{\mathcal{D}}{=} \frac{x^2}{x^2 + \sum_{i=1}^{K} Y_i},$$

where the $(Y_i)_{i\in\mathbb{N}}$ are i.i.d. copies of Y, K is Poisson(c)-distributed and independent of $(Y_i)_{i\in\mathbb{N}}$.

- The solution $Y(x)$ is reached parity-monotonically in the iterations.

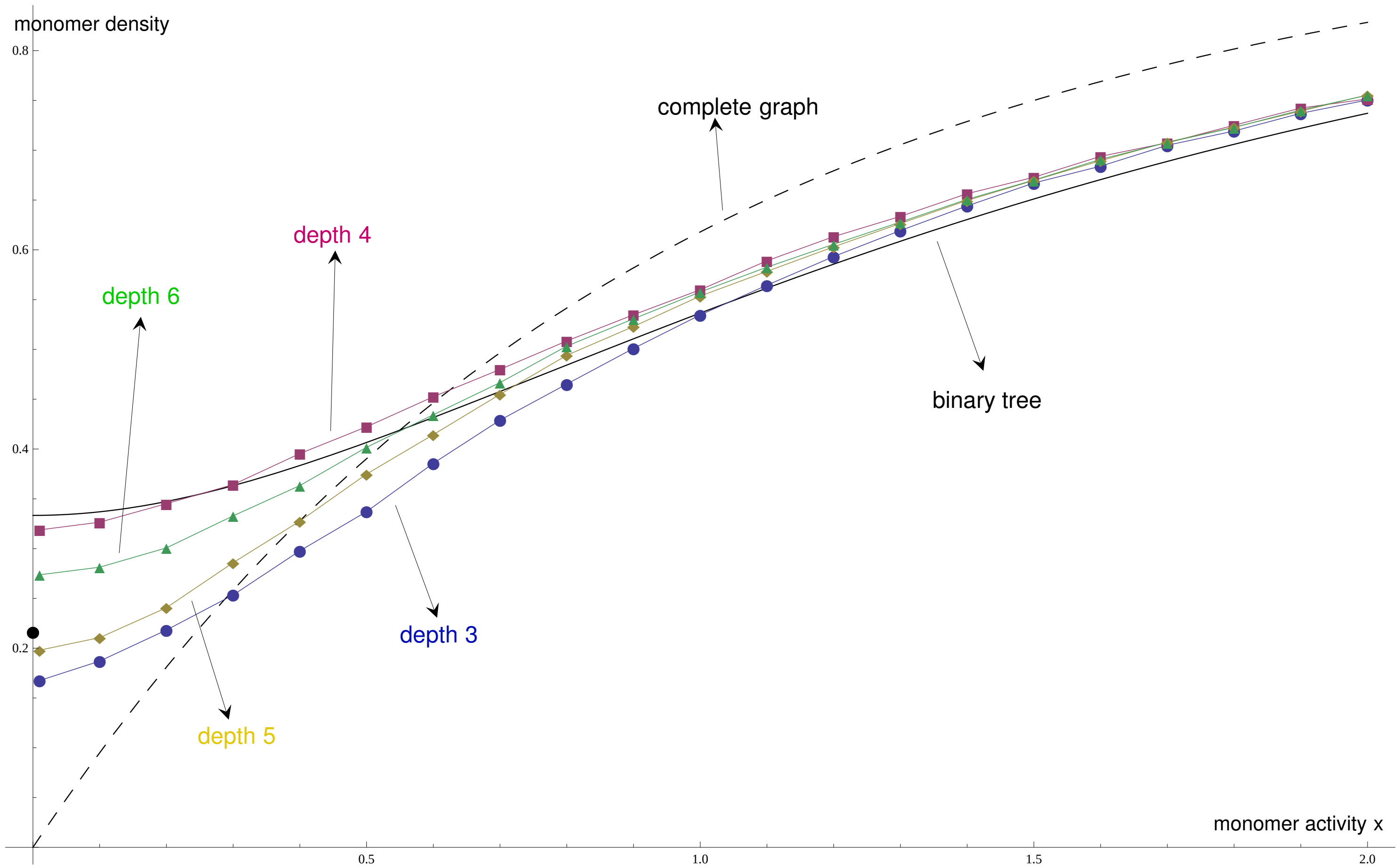
- Starting from $Y_i \equiv 1$, the even iterations decrease monotonically, the odd ones increase monotonically, their difference shrinks to zero and their common limit is an analytic function of x.

- the random monomer density converges almost surely, in the thermodynamic limit, to the analytic function:

$$\varepsilon(x) = \mathbb{E}(Y(x))$$

and the random pressure to

$$p(x) = -\,\mathbb{E}\Big[\log \frac{Y(x)}{x}\Big] - \frac{c}{2}\,\mathbb{E}\Big[\log\Big(1+\frac{Y_1(x)}{x}\,\frac{Y_2(x)}{x}\Big)\Big]\,.$$



Upper and lower bounds for the monomer density (c=2).

Proof Ideas

1) Analytic control of the probability of having a monomer in a vertex o: $\mathcal{R}_x(G, o)$

The Heilmann-Lieb identity translates into the relation

$$\mathcal{R}_x(G, o) = \frac{x^2}{x^2 + \sum_{v \sim o} \mathcal{R}_x(G - o, v)}$$

Theorem 1:

- The function $z \mapsto \mathcal{R}_z(G, o)$ is analytic on $\mathbb{C}_+$

- If $z \in \mathbb{C}_+$, then $|\mathcal{R}_z(G, o)| \leq |z| / \Re(z)$

2) Parity-alternating correlation inequalities for trees. Let $[G, o]_l$ be the ball of radius l and center o.

Theorem 2:

- If $[G, o]_{2r}$ is a tree, then $\mathcal{R}_x(G, o) \leq \mathcal{R}_x([G, o]_{2r}, o)$.
- If $[G, o]_{2r+1}$ is a tree, then $\mathcal{R}_x(G, o) \geq \mathcal{R}_x([G, o]_{2r+1}, o)$.

Morally: we show that odd and even iterations are monotonically convergent to analytic functions. Since the square iterated fixed point equation is a contraction for large values of x the two limits must coincide there and, by consequences of analyticity, everywhere.

Remarks

- Zdeborova and Mezard (2006) studied the problem for *sparse* random graphs and proposed an *exact* solution using the replica-symmetric cavity method.

- Also: C. Bordenave, M. Lelarge, J. Salez

Perspectives

- Diluted and Attractive

- Add random fields and random interactions, spin glass like...

- Computer science: belief propagation doesn't work anymore. Survey propagation enough?