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The exact solution of a mean-field monomer-dimer model with attractive potential

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Abstract – A monomer-dimer model with an attractive interaction that favors a phase separation between monomers and dimers is exactly solved in the mean-field case. With the identification of a suitable variational principle the free energy is computed in the large volume limit using the Heilmann-Lieb pure hard-core ansatz. The monomer density, that turns out to be the order parameter of the model, is shown to have a first-order phase transition along a coexistence curve.

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Monomer-dimer models were originally introduced to study the properties of diatomic oxygen molecules deposited on tungsten [1] or liquid mixtures with molecules of unequal size [2]. In these models the contact repulsion generated by the Pauli exclusion principle is realised through a topological constraint, the hard-core interaction, which forbids particles (monomers or dimers) to occupy the same site. In order to take into account also the attractive component of the van der Waals potential, one has to consider an attractive interaction [3–6] among dimers (as was previously done for single atoms [7,8]). An attractive potential can be added to a pure monomer-dimer model by assigning a higher probability to those configurations that have neighbouring sites occupied by similar molecules, either dimers or monomers. In this way those configurations where clusters of monomers are separated from clusters of dimers are favoured and a phase separation between monomers and dimers is expected to occur. The same modelling mechanism is used to study ferromagnetic systems where configurations with neighbouring aligned Ising spins are favoured and islands of positive spins are separated from those of negative spins at low temperatures.

Our work stems from the seminal contribution of Heilmann and Lieb [9,10], where the absence of phase transition in the case of pure hard-core dimer interaction was proved. While the addition of randomness on the topological structure of the graph was rigorously proved to induce no phase transitions for a large class of mean-field models [11], the addition of an attraction among similar particles is believed to generate a phase transition [3,7].

Heilmann and Lieb [5] indeed proved that, for certain finite-dimensional lattices, the attraction among dimers with the same orientation induces a phase transition.

In this letter we study the monomer-dimer model with attraction among similar particles in the complete graph and we find its exact solution. We compute the free energy in the thermodynamic limit as well as the order parameter of the theory which turns out to be the monomer density. We find that the model undergoes a first-order phase transition with the expected mean-field critical exponents.

The result we present here provides the first exact solution of a monomer-dimer system with an additional attractive interaction. Beside representing the mean-field approximation of physical theories in the lattice, our result is also interesting for the so-called matching problem in computer science [12–14] or for the newly emerging interdisciplinary applications of statistical-physics methods to the social sciences [15].

A monomer-dimer configuration on a finite graph G is a way to cover its edges by dimers and its vertices by monomers avoiding overlaps among them. In order to introduce an attractive interaction among similar particles, we start by observing that without loss of generality, for a regular graph G , the Hamiltonian of the model depends only on two parameters, h and $J > 0$. Its values on each configuration can be expressed as

$$-H_G \equiv hM + JI_m, \quad (1)$$

where M is the number of monomers and I_m is the number of couples of neighbouring monomers. This can be easily seen observing that, on any graph G , a general model

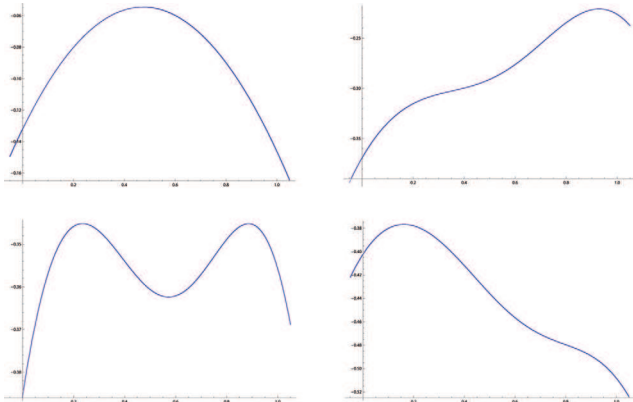


Fig. 1: (Colour on-line) The function \tilde{p} plotted *vs.* m , for different values of the parameters J and h . The considered values of (J, h) are, respectively, $(1, -0.9)$, $(3.5, -2)$, $(3.5, -2.1365)$, $(3.5, -2.3)$.

with attractive potential among particles is defined by the Hamiltonian

$$-H_G = h_m M + h_d D + J_m I_m + J_d I_d + J_{md} I_{md}, \quad (2)$$

where D is the number of dimers, I_d is the number of links between couples of dimers, I_{md} is the number of links between couples of molecules of different type. The parameters h_m, h_d tune, respectively, the presence of monomers and dimers; the parameters J_m, J_d, J_{md} tune, respectively, the attraction among monomers, among dimers and among different molecules. Denoting by N, L respectively the number of sites and links of the graph, it holds

$$M + 2D = N, \quad I_d + D + I_m + I_{md} = L; \quad (3)$$

hence the Hamiltonian (2) can be expressed, up to a constant, using only three parameters:

$$-H_G \equiv h'_m M + J'_m I_m + J'_d I_d \quad (4)$$

with $h'_m = h_m - \frac{1}{2}h_d + \frac{1}{2}J_{md}$, $J'_m = J_m - J_{md}$ and $J'_d = J_d - J_{md}$. When the graph is regular of degree r , it holds also

$$2I_m + I_{md} = rM; \quad (5)$$

therefore the Hamiltonian (4) turns out to be, up to a constant, eq. (1) with $h = h'_m - rJ'_d + \frac{1}{2}J'_d$ and $J = J'_m + J'_d$.

For the mean-field model, in order to have a well-defined thermodynamic limit (see [9]), the correct normalisation of the parameters in (1) with respect to the number of sites N is given by $h + \frac{1}{2} \ln N$ and J/N . The attractive nature of the potential among molecules of the same type is ensured by the condition $J \geq 0$.

The pressure (free energy up to a sign and a rescaling factor) of the model in the thermodynamic limit is

$$p = \lim_{N \rightarrow \infty} \frac{1}{N} \ln Z_N, \quad (6)$$

where Z_N is the partition function on the monomer-dimer configurations with Hamiltonian (1), conveniently normalized as described before. From the technical point of view

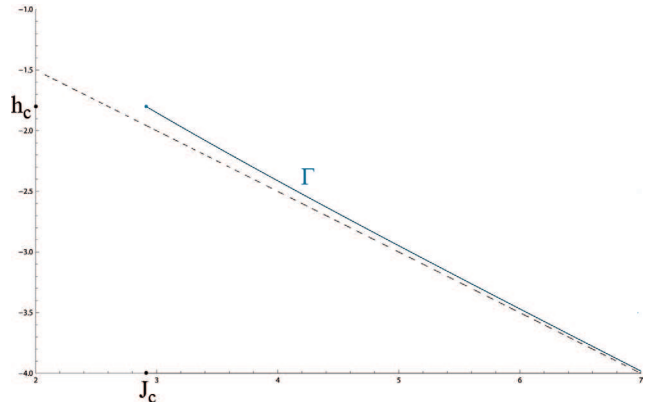


Fig. 2: (Colour on-line) The coexistence curve Γ , its asymptote and the critical point (J_c, h_c) represented on the half-plane (J, h) .

our main result is the identification of the following variational principle: considering $m \in [0, 1]$ one has

$$p = \sup_m \tilde{p}(m), \quad (7)$$

where the function \tilde{p} is

$$\tilde{p}(m) = -\frac{J}{2}m^2 + p^{\text{MD}}(Jm + h), \quad (8)$$

and p^{MD} is the pressure for the pure hard-core monomer-dimer model, *i.e.* $p^{\text{MD}}(\xi) = -\frac{1}{2}(1 - g(\xi)) - \frac{1}{2} \ln(1 - g(\xi))$ with $g(\xi) = \frac{1}{2}(\sqrt{e^{4\xi} + 4e^{2\xi}} - e^{2\xi})$. The explicit expression for p^{MD} can be derived (see [16] for the details) by an iterative equation found by Heilmann and Lieb in [9]. Using their ansatz, together with a variational principle developed within mean-field theories (see Guerra [17]), one can prove the two finite-volume lower and upper bounds

$$p_N^{\text{IMD}} \geq -\frac{J}{2}m^2 + p^{\text{MD}}\left(Jm + h - \frac{J}{2N}\right) \quad \forall m \in \mathbb{R},$$

$$p_N^{\text{IMD}} \leq \frac{\ln(N+1)}{N} + \sup_m \left\{ -\frac{J}{2}m^2 + p^{\text{MD}}\left(Jm + h - \frac{J}{2N}\right) \right\},$$

which immediately entail eq. (7) when the thermodynamic limit is considered.

The solution of the model reduces then to identify the value m^* that maximises \tilde{p} (the structure of this function is shown in fig. 1). Such value is found among the solutions of the consistency equation

$$m = g(Jm + h), \quad (9)$$

that include, beside the equilibrium value, also the unstable and metastable points. It is possible to prove (see [16] for details) that m^* (which represent the monomer density) is a smooth function for all the values of the parameters (J, h) with the exception of a coexistence curve Γ (see fig. 2). Γ is a differentiable curve in the half-plane

(J, h) which stems from the critical point

$$(J_c, h_c) = \left(\frac{3 + 2\sqrt{2}}{2}, \frac{1}{2} \ln(2\sqrt{2} - 2) - \frac{2 + \sqrt{2}}{2} \right) \quad (10)$$

and admits the asymptote

$$h + \frac{1}{2}J + \frac{1}{2} = 0. \quad (11)$$

It is possible to show that the function m^* is continuous but not differentiable at the critical point, while it has a jump discontinuity along the rest of the curve Γ .

The monomer density at the critical point is

$$m_c = 2 - \sqrt{2}. \quad (12)$$

The behaviour of m^* near the critical point is characterised by the following expansion:

$$(\xi - \xi_c)^3 - \kappa(J - J_c)(\xi - \xi_c) - J_c \kappa \rho = \mathcal{O}((\xi - \xi_c)^4),$$

where we have used the notations

$$\begin{aligned} \xi &= Jm^* + h, & \kappa &= \frac{3J_c}{2J}(2 - m_c), \\ \rho &= h - h_c + m_c(J - J_c). \end{aligned}$$

The critical exponents of m^* in the critical point, along the line of equation $a(h - h_c) = b(J - J_c)$ for $a, b \in \mathbb{R}$ not both zero, are

$$m^* - m_c \sim \begin{cases} \pm C_\Gamma (J - J_c)^{\frac{1}{2}}, & \text{if } b/a = -m_c \text{ and } J \geq J_c, \\ C_{b/a} (J - J_c)^{\frac{1}{3}}, & \text{if } b/a \neq -m_c \text{ and } a \neq 0, \\ C_\infty (h - h_c)^{\frac{1}{3}}, & \text{if } a = 0, \end{cases} \quad (13)$$

where

$$\begin{aligned} C_\Gamma &= \frac{1}{J_c} \sqrt{3(2 - m_c)}, \\ C_{b/a} &= \frac{1}{J_c} \sqrt[3]{\frac{3}{2} J_c (2 - m_c) \left(m_c + \frac{b}{a} \right)}, \\ C_\infty &= \frac{1}{J_c} \sqrt[3]{\frac{3}{2} J_c (2 - m_c)}. \end{aligned}$$

One can prove that the line determined by $b/a = -m_c$ coincides with the tangent of Γ at the critical point.

It would be interesting to investigate whether a similar method works also for the finite-dimensional cases for which an exact solution is known for the pure hard-core interaction, like the dimer (only) model in two dimensions (see [18]).

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