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Existence of Phase Transition for a Lattice Model with a Repulsive Hard Core and an Attractive Short Range Interaction

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Abstract. We consider a lattice model with a repulsive hard core and an attractive short range interaction. We show that this model has at least three independent equilibrium states, when the temperature is sufficiently low and the chemical potential is suitably chosen.

1. Introduction

The existence of a phase transition at sufficiently low temperature and/or high density has been proved for a large class of lattice models [1].

The procedure, now actually standard, goes back to Peierls [2] and relies in showing that the correlation functions are sensitive to boundary conditions even in the thermodynamic limit.

The fundamental steps are:

i) definition of contours: each configuration on a lattice is associated to a family of polygonals (the contours);

ii) estimate of an upper bound for the probability of finding a given contour present: this probability, in all cases of interest, turns out to decrease esponentially with the inverse temperature and the lenght of the contour.

The main difficulty generally arises in getting point ii) and, until recently, it was possible to get these sort of estimates only for systems exhibiting a symmetry.

A big progress has been recently achieved by Pirogov and Sinai [3], that were able to prove point ii) for an Ising spin system with small non symmetric perturbations[1].

In the present paper we consider a lattice model with a repulsive hard core and an attractive two-body short range interaction and, by the method of Peragov and Sinai, we show that there are at least three equilibrium states corresponding to different boundary conditions if the temperature is sufficiently low and the chemical potential is suitably chosen.

[1] The case where three-body interactions only are present, was solved by Merlini, Hintermann, and Gruber [4], in two dimensions with a different technique, based on duality transformations.

This model was previously studied by Dobrushin and shown to exhibit at least two indipendent non traslationally invariant equilibrium states, when the chemical potential is suitably large [5].

The calculation refers to the two dimensional case; generalisation to three or more dimensions does not present any particular difficulty.

In the second section we define the model and for suitable boundary conditions we express the partition functions in terms of contours. In the third section the Pirogov and Sinai method is applied. We conclude by briefly discussing a physical interpretation of our results and listing some obvious generalizations of our model.

2. The Model

Consider a box $\Lambda \subset \mathbb{Z}^2$, containing $|\Lambda|$ lattice points and call $\delta\Lambda$ its boundary. On each site $i \in \Lambda$ there is a spin variable $\sigma_i = \pm 1$ and $\boldsymbol{\sigma}_\Lambda \equiv (\sigma_1, \ldots, \sigma_{|\Lambda|})$ denotes an arbitrary configuration in Λ. The hamiltonian of the spin system we shall consider has the form

$$H(\boldsymbol{\sigma}_\Lambda) = \text{hard core} - J\sum_{\langle\langle i,J\rangle\rangle \in \Lambda} \sigma_i \sigma_J - h\sum_{i \in \Lambda} \sigma_i, \tag{2.1}$$

where the hard core acts between plus spins on nearest neighbours sites and the sum is over second neighbours pairs in Λ. If we split the lattice into the two sublattices $\mathbb{Z}_a^2$ and $\mathbb{Z}_b^2$, that connect second neighbours (cf. Fig. 1), with obvious notations $\Lambda = \Lambda_a \cup \Lambda_b$, $\boldsymbol{\sigma}_\Lambda = (\boldsymbol{\sigma}_{\Lambda_a} \cup \boldsymbol{\sigma}_{\Lambda_b})$, the hamiltonian will read

$$H(\boldsymbol{\sigma}_\Lambda) = \text{hard core} + H_I(\boldsymbol{\sigma}_{\Lambda_a}) + H_I(\boldsymbol{\sigma}_{\Lambda_b}), \tag{2.2}$$

where

$$H_I(\boldsymbol{\sigma}_{\Lambda_a}) = -J\sum_{\langle i,J\rangle \in \Lambda_a} \sigma_i \sigma_J - \cdot h\sum_{i \in \Lambda_a} \sigma_i \tag{2.3}$$

is the standard Ising hamiltonian with nearest neighbours interaction in the sublattice $\mathbb{Z}_a^2$.

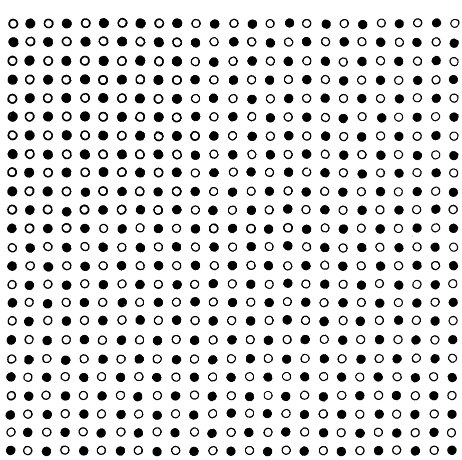

Fig. 1. ○ lattice $\mathbb{Z}_a^2$ ● lattice $\mathbb{Z}_b^2$

Now if we consider a box Λ, defined as in Fig. 2, we notice that all the sites $i \in \partial\Lambda$ belong to the same sublattice. Then, keeping all spins on $\partial\Lambda$ to be minus, we will focus our attention on the following two arrangements for all spins sitting on the sites internal to Λ and neighbouring $\partial\Lambda$:

i) they are all bound to be minus;

ii) they are all bound to be plus.

The first is what we call the τ_0 boundary conditions. For the second we have to distinguish two cases: $\partial\Lambda \in \mathbb{Z}_a^2$ and $\partial\Lambda \in \mathbb{Z}_b^2$ that we will denote respectively as τ_1 and τ_2 boundary conditions.

The thermodynamic limit will be taken over sequences, ordered by inclusion, of boxes $\{\Lambda\}$, preserving the boundary conditions.

We will now discuss in some detail the case of boundary conditions τ_1. If we call $\{\boldsymbol{\sigma}_\Lambda\}_\tau^6$ the set of all spin configurations in Λ, consistent with the hard core exclusion and boundary conditions τ_1, the partition sum over Λ will read:

$$Z^{\tau_1}(\Lambda, h, \beta) = \sum\nolimits_{\{\boldsymbol{\sigma}_\Lambda\}'_{\tau_1} = \{\boldsymbol{\sigma}_{\Lambda_a} \cup \boldsymbol{\sigma}_{\Lambda_b}\}'} e^{-\beta H_I^{(-)}(\boldsymbol{\sigma}_{\Lambda_a}) - \beta H_I^{(+)}(\boldsymbol{\sigma}_{\Lambda_b})}$$

where the superscript $+(-)$ in the hamiltonian is to recall the boundary conditions on each sublattice.

If we recall that any spin configuration $\boldsymbol{\sigma}_{\Lambda_a}(\boldsymbol{\sigma}_{\Lambda_b})$ is associated, by standard rules [6], to a polygonal separating opposite spins in the sublattice $\mathbb{Z}_a^2(\mathbb{Z}_b^2)$, we get that any $\boldsymbol{\sigma}_\Lambda \in \{\boldsymbol{\sigma}_\Lambda\}'_{\tau_1}$ can be associated to a collection of closed contours $\boldsymbol{\gamma} = \boldsymbol{\gamma}^{(a)} \cup \boldsymbol{\gamma}^{(b)}$, where:

i) the $\gamma^{(a)}$'s($\gamma^{(b)}$'s) are closed polygonals connecting adjacent points in the sublattice $\mathbb{Z}_a^2(\mathbb{Z}_b^2)$;

ii) two $\gamma^{(a)}$'s($\gamma^{(b)}$'s) cannot intersect by construction (once the convention for "chopping off" [7] the edges is assumed);

iii) a $\gamma^{(a)}$ and a $\gamma^{(b)}$ do not intersect due to the hard core exclusion;

iv) any contour $\gamma^{(a)}(\gamma^{(b)})$ defines a region $\theta(\gamma)$ in Λ with well defined boundary conditions (τ_1, τ_2 or τ_0) (cf. Fig. 2).

In the sequel we will express the partition function in terms of suitably chosen contours.

Given any configuration $\boldsymbol{\sigma}_\Lambda \in \{\boldsymbol{\sigma}_\Lambda\}'_{\tau_1}$, we can consider the associated contour configuration.

Among these contours, we can select the outer ones (i.e. the contours that are not embraced by any other contour); then we can collect the spin configurations $\boldsymbol{\sigma}_\Lambda$ in classes in the following way: all the $\boldsymbol{\sigma}_\Lambda$'s that give rise to the same outer contour configuration belong to the same class. Obviously a given $\boldsymbol{\sigma}_\Lambda \in \{\boldsymbol{\sigma}_\Lambda\}'_{\tau_1}$ cannot belong to different classes.

Notice that, due to the presence of the τ_1 boundary condition the outer contours can only be composed of pieces connecting adjacent points of the sublattice $\mathbb{Z}_a^2$.

Conversely let $\{\boldsymbol{\Gamma}^{(a)}\}_\Lambda$ be the set of all collections of compatible (i.e. not intersecting) outer contours of type $\gamma^{(a)}$ in Λ: then to any $\boldsymbol{\Gamma}^{(a)} \in \{\boldsymbol{\Gamma}^{(a)}\}_\Lambda$ we can associate all the spin configurations $\boldsymbol{\sigma}_\Lambda \in \{\boldsymbol{\sigma}_\Lambda\}_{\tau_1}$ that give rise to the outer contour configuration $\boldsymbol{\Gamma}^{(a)}$.

In this way we have partitioned the set $\{\boldsymbol{\sigma}_\Lambda\}_{\tau_1}$ in equivalence classes and we have constructed a one-to-one mapping from these classes onto the configuration $\boldsymbol{\Gamma}^{(a)} \in \{\boldsymbol{\Gamma}^{(a)}\}_\Lambda$.

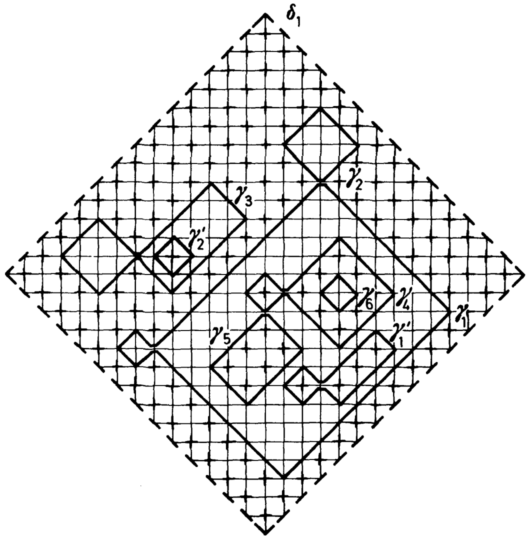

Fig. 2. Volume Λ with boundary conditions τ: a configuration γ_Λ and the associated set of contours $(\gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_5, \gamma_6, \gamma_1', \gamma_2')$. Notice that: (a) the γ's and the γ''s are polygonals connecting adjacent points in different sublattices; (b) the outer contours are $\gamma_1, \gamma_2, \gamma_3$; (c) $\gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_5, \gamma_6$, and $\partial\Lambda$ connect point in the same sublattice. For τ_0 boundary conditions see for instance the region $\theta(\gamma_1)$

Similar arguments $(a \to b)$ hold for τ_2 boundary conditions. The relevant difference for τ_0 boundary conditions is that we can simultaneously have outer contours belonging to different sublattices.

Let us set

$$\zeta^{\tau_1(\tau_2)}(\Lambda, h, \beta) = e^{-J\beta(\mathcal{N}_{\Lambda_a} + \mathcal{N}_{\Lambda_b}) \pm h\beta(|\Lambda_a| - |\Lambda_b|)} Z^{\tau_1(\tau_2)}(\Lambda, h, \beta)$$
$$\zeta^{\tau_0}(\Lambda, h, \beta) = e^{-J\beta(\mathcal{N}_{\Lambda_a} + \mathcal{N}_{\Lambda_b}) + h\beta|\Lambda|} Z^{\tau_0}(\Lambda, h, \beta),$$

where $\mathcal{N}_{\Lambda_a}(\mathcal{N}_{\Lambda_b})$ is the number of pairs of nearest neighbours on $\Lambda_a(\Lambda_b)$.

Then we can write:

$$\zeta^{\tau_1}(\Lambda, h, \beta) = \sum_{\boldsymbol{\Gamma}^{(a)} \in \{\boldsymbol{\Gamma}^{(a)}\}_\Lambda} \prod_{\Gamma^{(a)} \in \boldsymbol{\Gamma}^{(a)}} e^{-2\beta J|\Gamma^{(a)}| - 2\beta h|\theta(\Gamma^{(a)})|} \zeta^{\tau_0}(\theta(\Gamma^{(a)}), h, \beta), \tag{2.4}$$

$$\zeta^{\tau_2}(\Lambda, h, \beta) = \sum_{\boldsymbol{\Gamma}^{(b)} \in \{\boldsymbol{\Gamma}^{(b)}\}_\Lambda} \prod_{\Gamma^{(b)} \in \boldsymbol{\Gamma}^{(b)}} e^{-2\beta J|\Gamma^{(b)}| - 2\beta h|\theta(\Gamma^{(b)})|} \zeta^{\tau_0}(\theta(\Gamma^{(b)}), h, \beta), \tag{2.5}$$

$$\zeta^{\tau_0}(\Lambda, h, \beta) = \sum_{\boldsymbol{\Gamma}^{(a)} \cup \boldsymbol{\Gamma}^{(b)} \in \{\boldsymbol{\Gamma}^{(a)} \cup \boldsymbol{\Gamma}^{(b)}\}_\Lambda} \prod_{\Gamma^{(a)} \in \boldsymbol{\Gamma}^{(a)}} e^{-2\beta J|\Gamma^{(a)}| + 2\beta h|\theta(\Gamma^{(a)})|} \zeta^{\tau_1}(\theta(\Gamma^{(a)}), h, \beta)$$
$$\cdot \prod_{\Gamma^{(b)} \in \boldsymbol{\Gamma}^{(b)}} e^{-2\beta J|\Gamma^{(b)}| + 2\beta h|\theta(\Gamma^{(a)})|} \zeta^{\tau_2}(\theta(\Gamma^{(b)}), h, \beta) \tag{2.6}$$

where $\{\boldsymbol{\Gamma}^{(a)} \cup \boldsymbol{\Gamma}^{(b)}\}_\Lambda$ is the set of all collections of outer contours in Λ, $\boldsymbol{\Gamma}^{(a)} \cup \boldsymbol{\Gamma}^{(b)}$ such that no one of the $\Gamma^{(a)} \in \boldsymbol{\Gamma}^{(a)}$ intersects $a\Gamma^{(b)} \in \boldsymbol{\Gamma}^{(b)}$; $|\Gamma^{(a)}|(|\Gamma^{(b)}|)$ is the lenght of contour $\Gamma^{(a)}(\Gamma^{(b)})$ if we use the spacing of the sublattices as unit; $|\theta(\Gamma^{(a)})|(|\theta(\Gamma^{(b)})|)$ is the number of sites of $\Lambda_b(\Lambda_a)$ contained in the region $\theta(\Gamma^{(a)})(\theta(\Gamma^{(b)}))$.

3. The Method

Equations (2.4)–(2.6) of the previous sections show that the set of the allowed outer contour configurations and the associated outer contour wheights fully describe the model. Therefore all contour wheight functions that give rise to the same probability for outer contour configurations must be equivalent as far as the statistical behaviour of the system is concerned.

The phylosophy of Pirogov and Sinai's work is essentially based on the previous observation and their approach ammounts to look for contour wheight functions, consistent with the above mentioned requirements, that do satisfy the exponential bound quoted in point ii) of the introduction.

In the sequel we will reproduce the Pirogov and Sinai's argument for our model.

Let $\Omega_a(\Omega_b)$ be the set of all closed edge-self-avoiding contours in the sublattice $\mathbb{Z}_a^2(\mathbb{Z}_b^2)$ and $\Omega = \Omega_a \cup \Omega_b$. Introduce now $\mu^\tau(\gamma)$, $\mu^{\tau_b}(\gamma)$ two non negative, translationally invariant functions, defined on Ω and set:

$$\zeta^*(\mu^\tau, \Lambda) \begin{cases} = \sum_{\gamma^{(a)} \in \{\gamma^{(a)}\}_\Lambda} \prod_{\gamma^{(a)} \in \gamma^{(a)}} e^{-\mu^\tau(\gamma^{(a)})} = \sum_{\Gamma^{(a)} \in \{\Gamma^{(a)}\}_\Lambda} \prod_{\Gamma^{(a)} \in \Gamma^{(a)}} e^{-\mu^\tau(\Gamma^{(a)})} \zeta^*(\mu^\tau, \theta(\Gamma^{(a)})) \\ \quad \text{if} \quad \partial\Lambda \in \mathbb{Z}_a^2 \\ = \sum_{\gamma^{(b)} \in \{\gamma^{(b)}\}_\Lambda} \prod_{\gamma^{(b)} \in \gamma^{(b)}} e^{-\mu^\tau(\gamma^{(b)})} = \sum_{\Gamma^{(b)} \in \{\Gamma^{(b)}\}_\Lambda} \prod_{\Gamma^{(b)} \in \Gamma^{(b)}} e^{-\mu^\tau(\Gamma^{(b)})} \zeta^*(\mu^\tau, \theta(\Gamma^{(b)})) \\ \quad \text{if} \quad \partial\Lambda \in \mathbb{Z}_b^2 \end{cases} \tag{3.1}$$

$$\begin{aligned} \zeta(\mu^{\tau_0}, \Lambda) &= \sum_{\gamma^{(a)} \cup \gamma^{(b)} \in \{\gamma^{(a)} \cup \gamma^{(b)}\}_\Lambda} \prod_{\gamma^{(a)} \in \gamma^{(a)}} e^{-\mu^{\tau_0}(\gamma^{(a)})} \prod_{\gamma^{(b)} \in \gamma^{(b)}} e^{-\mu^{\tau_0}(\gamma^{(b)})} \\ &= \sum_{\Gamma^{(a)} \cup \Gamma^{(b)} \in \{\Gamma^{(a)} \cup \Gamma^{(b)}\}_\Lambda} \prod_{\Gamma^{(a)} \in \Gamma^{(a)}} {}^{-\mu^{\tau_0}(\Gamma^{(a)})} \zeta(\mu^{\tau_0}, \theta(\Gamma^{(a)})) \\ &\quad \cdot \prod_{\Gamma^{(b)} \in \Gamma^{(b)}} e^{-\mu^{\tau_0}(\Gamma^{(b)})} \zeta(\mu^{\tau_0}, \theta(\Gamma^{(b)})), \end{aligned} \tag{3.2}$$

where the star is to recall that only contour configurations $\gamma \in \Omega_a(\gamma \in \Omega_b)$ are taken in the sum (3.1).

We will prove the following theorem in order to show that our model exhibits a phase transition.

Theorem. *Consider the system described by Eqs.* (2.4)–(2.6) *of Section* 2. *When* $\frac{\beta J}{2} > e^{-\frac{\beta J}{2}}$ *it is possible to find a value of* h, $h^* = h^*(\beta, J)$, *for which there exist two wheight functions* $\mu^\tau(\gamma)$ *and* $\mu^{\tau_0}(\gamma)$ *such that:*

i) $\zeta^*(\mu^\tau, \theta(\gamma)) = \begin{cases} \zeta^{\tau_1}(h^*, \beta, \theta(\gamma)) & \text{for} \quad \gamma \in \Omega_a \\ \zeta^{\tau_2}(h^*, \beta, \theta(\gamma)) & \text{for} \quad \gamma \in \Omega_b \end{cases}$

$\zeta(\mu^{\tau_0}, \theta(\gamma)) = \zeta^{\tau_0}(h^*, \beta, \theta(\gamma)) \; \forall \, \gamma \in \Omega$.

ii) $$\mu^\tau(\gamma) - \ln \zeta^*(\mu^\tau, \theta(\gamma)) = 2\beta J|\gamma| + 2h\beta|\theta(\gamma)| - \ln \zeta(\mu^{\tau_0}, \theta(\gamma)) \tag{3.3}$$
$$\mu^{\tau_0}(\gamma) - \ln \zeta(\mu^{\tau_0}, \theta(\gamma)) = 2\beta J|\gamma| - 2h\beta|\theta(\gamma) - \ln \zeta^*(\mu^\tau, \theta(\gamma)). \tag{3.4}$$

iii) $\mu^\tau(\gamma) \geqq 2\beta J|\gamma|$

$\mu^{\tau_0}(\gamma) \geqq 2\beta J|\gamma|$.

Proof. If we set:

$$\ln \zeta^*(\mu^\tau, \theta(\gamma)) = 2|\theta(\gamma)|\alpha^*(\mu^\tau) + K^*(\mu^\tau, \theta(\gamma))$$

$$\ln \zeta(\mu^{\tau_0}, \theta(\gamma)) = 2|\theta(\gamma)|\alpha(\mu^{\tau_0}) + K(\mu^{\tau_0}, \theta(\gamma))$$

for $h = [\alpha(\mu^{\tau_0}) - \alpha^*(\mu^\tau)]/\beta$

the Eqs. (3.3) and (3.4) become

$$\boldsymbol{M}=\boldsymbol{A}+\boldsymbol{K}(\boldsymbol{M}),$$

where

$$\boldsymbol{M}=\begin{pmatrix}\mu^{\tau}(\gamma)\\ \mu^{\tau o}(\gamma)\end{pmatrix}$$

$$\boldsymbol{A}=\begin{pmatrix}2\beta J|\gamma|\\ 2\beta J|\gamma|\end{pmatrix}$$

$$\boldsymbol{K}(\boldsymbol{M})=\begin{pmatrix}K^*(\mu^{\tau},\theta(\gamma))-K(\mu^{\tau o},\theta(\gamma))\\ K(\mu^{\tau o},\theta(\gamma))-K^*(\mu^{\tau},\theta(\gamma))\end{pmatrix}.$$

Putting now:

$$\boldsymbol{M}_0=\boldsymbol{A}$$

$$\boldsymbol{M}_n=\boldsymbol{A}+\boldsymbol{K}(\boldsymbol{M}_{n-1})$$

by means of a theorem due to Minlos and Sinai [8], it is possible to show by standard methods (cf. Ref. [3]), that, when $\frac{\beta J}{2}>e^{-\frac{\beta J}{2}}$

$$\lim_{n\to\infty}\boldsymbol{M}_n=\boldsymbol{M}^*$$

exists for all γ's and $\boldsymbol{M}^*$ is the searched solution, h^* is then given by Eq. (3.6).

To conclude the proof we remark that for any γ which cannot contain internal contours

$$\zeta^{\tau}(h^*,\beta,\theta(\gamma))=\zeta^*(\mu^{\tau},\theta(\gamma))=1$$

and by interation it is easy to prove point i), of our theorem, for any γ.

4. Conclusions

We have shown that when $\frac{\beta J}{2}>e^{-\frac{\beta J}{2}}$ and $h=h^*(\beta,J)$, we have at least three independent states associated, respectively, to the outer contour probability distributions, given by the contour wheight functions μ^{τ}, $\mu^{\tau o}$.

If we remark that the states with τ_1 and τ_2 boundary conditions are not translationally invariant, it seems natural, in the language of the lattice gas, to interpret the curve $h=h^*(\beta,J)$ as the solid-fluid transition line. It would be nice to be able to discriminate between two fluid phases and get the full picture of a solid-fluid system. But this is far from the purposes and limits of this work and, presumably, the model is too simple to exibit this behaviour. A more feasible problem is to extend these results to longer range forces. For instance the case of first and second neighbours hard core exclusion and third neighbours attraction can be treated exactly along the same lines, and only minor changes are required when the third neighbours attraction is replaced by a longer range interaction à la Ginibre, Grossmann, and Ruelle [9]. Nevertheless the extension to arbitrary ranges is not obvious.

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