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ONE-DIMENSIONAL NON-SYMMETRIC WIDOM–ROWLINSON MODEL WITH LONG-RANGE INTERACTION

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The absence of phase transitions in one-dimensional Widom–Rowlinson model with long-range interaction is established in the non-symmetric case when different particles have different activity parameters.

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1. Introduction and Formulation of Results

Many multicomponent fluids are situated in a single phase because of a gain in mixing entropy. The system may possibly go to demixing if some thermodynamical variables change. One of the basic mechanisms explaining this kind of phase separations lies in the relative strengths of repulsion between like and unlike particles: if the unlike particles experience a stronger repulsion than the like ones, at least at high density demixing phases are favored. The prototype for analogous systems is the Widom–Rowlinson model. The two-particle Widom–Rowlinson model is a lattice gas model with two types of particles, allowed to sit on neighboring sites only if they are of the same type. Originally, the model was introduced[1] as a continuum model of particles living in $\mathbf{R^n}$. The lattice variant was studied firstly.[2] The spin variables $\phi(x)$ belong to the spin space $\Phi = \{-1, 0, +1\}$, where -1 and $+1$ are particle types and 0 corresponds to empty sites. The Hamiltonian of the model is defined as

$$H_0(\phi) = \sum_{x \in \mathbf{Z}^d} U_0(\phi(x)) + \sum_{x,y \in \mathbf{Z}^d} U_1(\phi(x), \phi(y)) \,, \qquad (1)$$

where the chemical potential

$$U_0(\phi(x)) = \begin{cases} -\ln \lambda_- & \text{if } \phi(x) = -1 \,, \\ 0 & \text{if } \phi(x) = 0 \,, \\ -\ln \lambda_+ & \text{if } \phi(x) = +1 \,. \end{cases}$$

$\lambda_- > 0$ and $\lambda_+ > 0$ are the activity parameters of particles -1 and $+1$ and the hard-core pair interaction is given by

$$U_1(\phi(x), \phi(y)) = \begin{cases} \infty & \text{if } \phi(x)\phi(y) = -1 \quad \text{and} \quad |x - y| = 1\,, \\ 0 & \text{otherwise}\,. \end{cases}$$

This hard-core model exhibits so-called hard constraints, meaning that their properties arise by forbidding certain configurations. The model is similar to the Ising model: for small values of $\beta\lambda_- = \beta\lambda_+$, there is a unique Gibbs state on which the overall density of $+1$ particles is almost surely equal to that of -1 particles. At $d \geq 2$ and for sufficiently large values of $\beta\lambda_- = \beta\lambda_+$, the symmetry of -1 and $+1$ particles is broken: there are limiting Gibbs states with overwhelming densities of -1 and $+1$ particles. In non-symmetric case $\lambda_- \neq \lambda_+$ in $d \geq 2$ most likely limiting Gibbs state is unique, but rigorous proof is not known. In this paper, we deal with the non-symmetric case for $d = 1$.

Consider the one-dimensional long-range Widom–Rowlinson model with the Hamiltonian

$$H(\phi) = \sum_{x \in \mathbf{Z}^1} U_0(\phi(x)) + \sum_{x,y \in \mathbf{Z}^1} U_1(\phi(x), \phi(y)) + \sum_{x,y \in \mathbf{Z}^1} U_2(\phi(x), \phi(y))\,, \tag{2}$$

where

$$U_2(\phi(x), \phi(y)) = \begin{cases} -|x - y|^{-\alpha} & \text{if } \phi(x)\phi(y) = 1\,, \\ 0 & \text{otherwise}\,. \end{cases}$$

The parameter α satisfies the natural condition $\alpha > 1$ necessary for the existence of the thermodynamic limit.

In this paper, we investigate the problem of uniqueness of Gibbs states of the model (2). If $\alpha > 2$, then the uniqueness of Gibbs states directly follows from the well-known uniqueness condition for one-dimensional models. This condition states that the interaction between very distant spins should decrease so rapidly that the total interaction energy of the spins on any two complementary half-lines is finite.[3–5] In other words, the model satisfying the condition $\sum_{r \in \mathbf{Z}^1, r > 0} r|U(r)| < \infty$ ($U(r)$ is a pair potential of long range) has a unique limiting Gibbs state.[3,5] The very problem arises in the case $2 > \alpha > 1$ when $\sum_{r \in \mathbf{Z}^1, r > 0} r|U(r)| = \infty$. In the symmetric case $\lambda_- = \lambda_+$ the model may exhibit a phase transition at low temperatures similar to the ferromagnetical Ising model with long range interaction,[6,7] but the rigorous proof is not known. Since the model (2) has strong long-range interaction ($2 > \alpha$) the general methods[3–5] does not work. Below, we consider non-symmetric case $\lambda_- \neq \lambda_+$ and by using of special method developed in elsewhere[8] prove the uniqueness of limiting Gibbs states at low temperatures:

Theorem 1. *For each values of λ_- and λ_+ such that $\lambda_- \neq \lambda_+$ a value of the inverse temperature β_{cr} exists such that if $\beta > \beta_{cr}$ then the model* (2) *has at most one limiting Gibbs state.*

2. Proofs

In order to prove Theorem 1, we use a method which reduces the problem of uniqueness of limiting Gibbs states to the problem of percolation of special clusters.[8]

A configuration ϕ^{gr} is said to be a ground state, if for any finite perturbation ϕ' of the configuration ϕ^{gr}, the expression $H(\phi') - H(\phi^{gr})$ is non-negative.

Below $\phi(B)$ denotes the restriction of the configuration ϕ to the set B. We say that the ground state ϕ^{gr} of the model (1) satisfies the Peierls stability condition, if a constant t exists such that for any finite set $A \subset \mathbf{Z}^1$ $H(\phi') - H(\phi^{gr}) \geq t|A|$, where $|A|$ denotes the number of sites of A and ϕ' is a perturbation of ϕ^{gr} on the set A.

Without loss of generality, we suppose that $\lambda_+ > \lambda_-$.

Lemma 1. *For each values of λ_- and λ_+ such that $\lambda_- \neq \lambda_+$ the model* (2) *has a unique ground state ϕ^{gr} satisfying Peierls stability condition.*

Proof. Proof readily follows from the definitions with constant configuration $\phi^{gr} = 1$ and $t = \ln \lambda_+$.

Let V_N be an interval with the center at the origin and with the length of edge $2N$. The set of all configurations $\phi(V_N)$ we denote by $\Phi(N)$. Suppose that the boundary conditions $\phi^i, i = 1,2$ are fixed. Let $\mathbf{P}^{\mathbf{i}}_{\mathbf{N}}$ be the Gibbs distribution on $\Phi(N)$ corresponding to the boundary conditions ϕ^i, $i = 1,2$. Take $M < N$ and let $\mathbf{P}^{\mathbf{i}}_{\mathbf{N}}(\phi'(V_M)$ be the probability of the event that the restriction of the configuration $\phi(V_N)$ to V_M coincides with $\phi'(V_M)$.

The concatenation of the configurations $\phi(V_N)$ and $\phi^i(\mathbf{Z}^1 - V_N)$, we denote by χ: $\chi(x) = \phi(x)$, if $x \in V_N$ and $\chi(x) = \phi^i(x)$, if $x \in \mathbf{Z}^1 - V_N$. Define

$$H_N(\phi|\phi^i) = \sum_{B \subset \mathbf{Z}^1 : B \cap V_N \neq \emptyset} U(\chi(B)) .$$

The set of configurations with minimal energy at fixed N and boundary conditions ϕ^i, we denote by $\Phi^{\min}(N, \phi^i)$. Let $\phi_N^{\min,i}$ be an arbitrarily chosen representative of this set:

$$H_N(\phi_N^{\min,i}|\phi^i) = \min_{\phi \in \Phi(N)} H_N(\phi|\phi^i) .$$

Let $H_N(\phi|\phi^i, \phi_N^{\min,i})$ be the relative energy of a configuration ϕ (with respect to $\phi_N^{\min,i}$):

$$H_N(\phi|\phi^i, \phi_N^{\min,i}) = H_N(\phi|\phi^i) - H_N(\phi_N^{\min,i}|\phi^i) .$$

By Lemma 1 the ground state of the model (2) is unique and therefore the configuration $\phi_N^{\min,i}$ almost coincides with the ground state φ^{gr}.[9]

Let $\mathbf{P}^{\mathbf{i}}_{\mathbf{N}}$ be Gibbs distributions on $\Phi(N)$ corresponding to the boundary conditions ϕ^i, $i = 1,2$ defined by using of relative energies of configurations. Take $M < N$ and let $\mathbf{P}^{\mathbf{i}}_{\mathbf{N}}(\phi'(V_M)$ be the probability of the event that the restriction of the configuration $\phi(V_N)$ to V_M coincides with $\phi'(V_M)$.

Suppose that the boundary conditions ϕ^1 are fixed. Consider the $\mathbf{P}_N^1$ probability of the event that the restriction of the configuration $\phi(V_N)$ to V_M coincides with $\phi'(V_M)$:

$$\mathbf{P}_N^1(\phi'(V_M)) = \frac{\sum_{\phi(V_N):\phi(V_M)=\phi'(V_M)} \exp(-\beta H_N(\phi(V_N)|\phi^1, \phi_N^{\min,1}))}{\sum_{\phi(V_N)} \exp(-\beta H_N(\phi(V_M)|\phi^1, \phi_N^{\min,1}))}$$

$$= \frac{\exp(-\beta H_M^{in}(\phi'(V_M)))Y(\phi'(V_M), V_N, \phi^1)\Xi(V_N - V_M|\phi^1, \phi'(V_M), \phi_N^{\min,1})}{\sum_{\phi''(V_M)} \exp(-\beta H_M^{in}(\phi''(V_M)))Y(\phi''(V_M), V_N, \phi^1)\Xi(V_N - V_M|\phi^1, \phi''(V_M), \phi_N^{\min,1})}$$

$$= \frac{\exp(-\beta H_M^{in}(\phi'(V_M)))Y(\phi'(V_M), V_N, \phi^1)\Xi^{\phi^1,\phi'}}{\sum_{\phi''(V_M)} \exp(-\beta H_M^{in}(\phi''(V_M)))Y(\phi''(V_M), V_N, \phi^1)\Xi^{\phi^1,\phi''}}\,, \tag{3}$$

where the summation in $\sum_{\phi''(V_M)}$ is taken over all possible configurations $\phi''(V_M)$, $H_M^{in}(\phi'(V_M)) = \sum_{B\subset V_M}\sum_{i=0}^2(U_i(\phi'(B)) - U_i(\phi_N^{\min,1}))$ and $H_M^{in}(\phi''(V_M)) = \sum_{B\subset V_M}\sum_{i=0}^2(U_i(\phi''(B)) - U_i(\phi_N^{\min,1}))$ are interior relative energies of $\phi'(V_M)$ and $\phi''(V_M)$. $\Xi^{\phi^1,\phi'}$ and $\Xi^{\phi^1,\phi''}$ denote the partition functions corresponding to the boundary conditions $\phi^1(\mathbf{Z}^\nu - V_N), \phi'(V_M), \phi''(V_M)$:

$$\Xi^{\phi^1,\phi'} = \Xi(V_N - V_M|\phi^1, \phi'(V_M), \phi_N^{\min,1}),\;\; \Xi^{\phi^1,\phi''} = \Xi(V_N - V_M|\phi^1, \phi''(V_M), \phi_N^{\min,1})\,. \tag{4}$$

The factor $Y(\phi(V_M), V_N, \phi^1)$ is defined as

$$Y(\phi(V_M), V_N, \phi^1) = \prod_{A\subset\mathbf{Z}^1:A\cap V_M\neq\emptyset;A\cap\mathbf{Z}^1-V_N\neq\emptyset;A\cap V_N-V_M=\emptyset} \exp(-\beta(U_2(\phi(A)) - U_2(\phi_N^{\min,1}(A)))) \tag{5}$$

where ϕ in (5) is equal to ϕ' for $x \in V_M$ and is equal to ϕ^1 for $x \in \mathbf{Z}^1 - V_N$.

Let us consider the partition functions $\Xi^{\phi^1,\phi''} = \Xi(V_N - V_M|\phi^1, \phi''(V_M), \phi_N^{\min,1})$ corresponding to the boundary conditions $\phi^1(\mathbf{Z}^1 - V_N)$, $\phi''(V_M)$ and $\Xi^{\phi^2,\phi'} = \Xi(V_N - V_M|\phi^2, \phi'(V_M), \phi_N^{\min,2})$ corresponding to the boundary conditions $\phi^2(\mathbf{Z}^\nu - V_N)$, $\phi'(V_M)$ as in (4).

Now define a super partition function

$$(\Xi^{\phi^1,\phi''}\;\; \Xi^{\phi^2,\phi'}) = \sum \exp(-\beta H_N(\phi^3(V_N)|\phi^1, \phi'', \phi_V^{\min,1}))\exp(-\beta H_N(\phi^4(V_N)|\phi^2, \phi', \phi_N^{\min,2}))\,,$$

where the summation is taken over all pairs of configurations $\phi^3(V_N)$ and $\phi^4(V_N)$, such that $\phi^3(V_M) = \phi''(V_M), \phi^4(V_M) = \phi'(V_M)$.

Consider the partition of $\mathbf{Z}^1$ into intervals $V(x)$, where $V(x)$ is an interval with an edge length 1 and with its center at x, where $x = 1/2 + k$; k is an integer number.

Let us consider an arbitrary configuration ϕ. We say that an interval $V(x)$ is not regular, if $\phi(V_R(x)) \neq \phi^{gr}(V_R(x))$. Two non-regular intervals are called connected provided that their intersection is not empty. The connected components of non-regular intervals defined in this way are called supports of contours and are denoted by $\operatorname{supp} K$.

A pair $K = (\operatorname{supp} K, \phi(\operatorname{supp} K))$ is called a contour.

Obviously for each contour K, a configuration ψ_K exists such that the only contour of the configuration ψ_K is K (ψ_K on $\mathbf{Z}^1 - \operatorname{supp} K$ coincides with ϕ^{gr}).

The statistical weight of a contour is

$$w(K_i) = \exp(-\beta(H(\psi_{K_i}) - H(\phi^{gr}))) \,. \tag{6}$$

The following equation is a direct consequence of (6):

$$\exp(-\beta H_N(\phi|\phi^1, \phi_N^{\min,1}) = \prod_{i=1}^{n} w(K_i) \exp(-\beta G(K_1, \ldots, K_n)) \,, \tag{7}$$

where the multiplier $G(K_1, \ldots, K_n)$ corresponds to the interaction between contours and with the boundary conditions ϕ^1.

$$G(K_1, \ldots, K_n) = \sum_{k=2}^{n} \sum_{i_1,\ldots,i_k} G(K_{i_1}, \ldots, K_{i_k}) \,, \tag{8}$$

where at each fixed k the summation is taken over all possible non-ordered collections $i_1, \ldots, i_k$.

The interaction between $K_{i_1}, \ldots, K_{i_k}$ arises due to the fact that the weight of the contour $K_{i_j}, j = 1, \ldots, k$ was calculated under assumption that the configuration outside $\operatorname{supp}(K_{i_j})$ coincides with the ground state.

The set of all interaction terms in the double sum (8) will be denoted by IG. Now we write (7) as follows:

$$\begin{aligned}\exp(-\beta H_N(\phi|\phi^1, \phi_N^{\min,1})) &= \prod_{i=1}^{n} w(K_i) \prod_{B\in IG} (\exp(-\beta G(K_{i_1}, \ldots, K_{i_k}))) \\ &= \prod_{i=1}^{n} w(K_i) \prod_{G\in IG} (1 + \exp(-\beta G(K_{i_1}, \ldots, K_{i_k}) - 1)) \,. \end{aligned} \tag{9}$$

From (9) we get

$$\exp(-\beta H(\phi|\phi^1, \phi_N^{\min,1}) = \sum_{IG'\subset IG} \prod_{i\in\mathbf{I}} w(K_i) \prod_{G\in IG'} g(G) \,, \tag{10}$$

where the summation is taken over all subsets IG' (including the empty set) of the set IG, and $g(G) = \exp(-\beta G) - 1$.

Consider an arbitrary term of the sum (10), which corresponds to the subset $IG' \subset IG$. Let the interaction element $G \in IG'$. Consider the set $\mathbf{K}$ of all contours such that for each contour $K \subset \mathbf{K}$, the set $\operatorname{supp} K \bigcap G$ is nonempty. We call any two contours from $\mathbf{K}$ neighbors in IG' interaction. The set of contours K' is called connected in IG' interaction if for any two contours K_p and K_q there exists a collection $(K_1 = K_p, K_2, \ldots, K_n = K_q)$ such that any two contours K_i and $K_{i+1}, i = 1, \ldots, n-1$, are neighbors.

The pair $D = [(K_i, i = 1, \ldots, s); IG']$, where IG' is some set of interaction elements, is called a cluster provided there exists a configuration ϕ containing all $K_i; i = 1, \ldots, s; IG' \subset IG$; and the set $(K_i, i = 1, \ldots, s)$ is connected in IG' interaction. The statistical weight of a cluster D is defined by the formula

$$w(D) = \prod_{i=1}^{s} w(K_i) \prod_{(x,y)\in IG'} g(G)\,.$$

Two clusters D_1 and D_2 are called compatible provided any two contours K_1 and K_2 belonging to D_1 and D_2, respectively, are compatible. A set of clusters is called compatible provided any two clusters of it are compatible.

If $D = [(K_i, i = 1, \ldots, s); IG']$, then we say that $K_i \in D; i = 1, \ldots, s$.

If $[D_1, \ldots, D_m]$ is a compatible set of clusters and $\bigcup_{i=1}^{m} \operatorname{supp} D_i \subset V_N$, then there exists a configuration ϕ which contains this set of clusters. For each configuration ϕ we have

$$\exp(-\beta H_N(\phi|\phi^1, \phi_N^{\min,1})) = \sum_{IG'\subset IG} \prod w(D_i)\,,$$

where the clusters D_i are completely determined by the set IG'. The partition function is

$$\Xi(\phi^1) = \sum w(D_1)\cdots w(D_m)\,,$$

where the summation is taken over all non-ordered compatible collections of clusters.

Since the model (2) has long-range interaction, contours interact, but above defined clusters do not interact if the have no intersection.[10]

The following generalization of the definition of compatibility allows us to represent $(\Xi^{\phi^1,\phi''}\,\Xi^{2,'})$ as a single partition function.

A set of clusters is called 2-compatible provided any of its two parts coming from two Hamiltonians is compatible. In other words, in 2-compatibility an intersection of supports of two clusters coming from different partition functions is allowed.

If $[D_1, \ldots, D_m]$ is a 2-compatible set of clusters and $\bigcup_{i=1}^{m} \operatorname{supp} D_i \subset V_N - V_M$, then there exist two configurations ϕ^3 and ϕ^4 which contain this set of clusters. For each pair of configurations ϕ^3 and ϕ^4 we have

$$\exp(-\beta H_N(\phi^3|\phi^1, \phi_N^{\min,1})\exp(-\beta H_N(\phi^4|\phi^2, \phi_N^{\min,2}) = \sum_{IG'\subset IG, IG''\subset IG} \prod w(D_i)\,,$$

where the clusters D_i are completely determined by the sets IG' and IG''.

The double partition function is

$$\Xi^{\phi^1,\phi'',\phi^2,\phi'} = \Xi^{\phi^1,\phi''} \qquad \Xi^{\phi^2,\phi'} = \sum w(D_1)\cdots w(D_m)$$

where the summation is taken over all non-ordered 2-compatible collections of clusters.

Let $w(D_1), \ldots, w(D_m)$ be a term of the double partition function $\Xi^{\phi^1,\phi'',\phi^2,\phi'}$. The connected components of the collection $[\text{supp}(D_1), \ldots, \text{supp}(D_m)]$ are the supports of the general clusters. A general cluster SD is a pair $(\text{supp}(SD), \phi(\text{supp}(SD))$. Below, instead of the expression "generally compatible collection of clusters" we use the expression "compatible collection of 2-clusters".

A 2-cluster $SD = [(D_i, i = 1, \ldots, m); IG', IG'']$ is said to be long if the intersection of the set $(\bigcup_{i=1}^{m} \text{supp}\, D_i) \bigcup IG' \bigcup IG''$ with both V_M and $\mathbf{Z}^\nu - V_N$ is nonempty. In other words, a long 2-cluster by using of its contours and bonds connects the boundary with the cube V_M.

A set of 2-clusters is called compatible provided the set of all clusters belonging to these 2-clusters are 2-compatible.

We say that the model (1) has not-long 2-clusters property, if a number $\epsilon, 0 < \epsilon < 1$ exists such that for each fixed cube V_M, a number $N_0 = N_0(M)$, which depends on M only exists such that if $N > N_0$, then

$$(1-\epsilon)\Xi^{\phi^1,\phi',\phi^2,\phi''} < \Xi^{\phi^1,\phi',\phi^2,\phi'',(n.l.)} = \sum w(SD_1)\cdots w(SD_m) < (1+\epsilon)\Xi^{\phi^1,\phi',\phi^2,\phi''}\,, \quad (11)$$

where the summation is taken over all non-long, non-ordered compatible collections of 2-clusters $[SD_1, \ldots, SD_m], \bigcup_{i=1}^{m} \text{supp}(SD_i) \subset V_N - V_M$ corresponding to the boundary conditions $\{\phi^1(\mathbf{Z}^1 - V_N), \phi^2(\mathbf{Z}^1 - V_N); \phi'(V_M)$ and $\phi''(V_M)\}$.

By definitions, in models with not-long 2-clusters property the statistical weights of long 2-clusters are negligible.

We are ready to formulate the uniqueness criterion:

Theorem 2. *Any model* (1) *having not-long* 2*-clusters property has at most one limiting Gibbs state.*

Theorem 2 has an application to some one-dimensional models[9]:

Theorem 3. *Suppose that a one-dimensional model has a unique ground state satisfying Peierls stability condition and a constant $\gamma < 1$ exists such that for any number L and any interval $I = [a, b]$ with length n and for any configuration $\phi(I)$*

$$\sum_{B\subset Z^1; B\cap I\neq\emptyset, B\cap(Z^1-[a-L,b+L])\neq\emptyset} |U(B)| \leq const\, n^\gamma\, L^{\gamma-1}\,. \quad (12)$$

A value of the inverse temperature β_{cr} exists such that if $\beta > \beta_{cr}$ then the model has at most one limiting Gibbs state.

We complete the proof of Theorem 1 by applying of Theorem 3. Indeed, by Lemma 1 the ground state ϕ^{gr} is unique and stable, and the condition $|U_2(\phi(x), \phi(y)| \leq |x-y|^{-\alpha}$ with $\alpha > 1$ readily implies (12).

3. Final Remarks

In ferromagnetical Ising model with long-range interaction at law temperatures there are at least two limiting Gibbs states corresponding to $+1$ and -1 particles[6,7]: for arbitrary large volume boundary particles outside this volume support like particles inside the volume. Theorem 1 shows that in non-symmetric Widom–Rowlinson model the ferromagnetical influence of the boundary particles on like particles inside the volume disappears while volume grows: in a chain of two particles, if adjacent sites cannot be occupied simultaneously by unlike particles, in spite of very long-range attraction potential between like particles, the phase inside sufficiently large volume is independent on the configuration outside the volume.

Most likely the uniqueness of limiting Gibbs states at non symmetric case is valid at all values of the temperature. Since the main method[8,9] used in this paper works only at low temperatures Theorem 1 is proved at low temperature regime.

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