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The Structure of Gibbs States and Phase Coexistence for Non-Symmetric Continuum Widom Rowlinson Models*

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Summary. We prove the existence of phase transitions in non-symmetric r-component continuum Widom-Rowlinson models. Our results are based on an extension of the Pirogov-Sinai theory of phase transitions in general lattice spin systems to continuum systems. This generalizes Ruelle's extension of the Peierls argument for lattices to symmetric continuum Widom-Rowlinson models. The Pirogov-Sinai picture of the low temperature phase diagram for spin systems goes over into a phase-diagram of the Widom-Rowlinson model at large fugacities $z=(z_0, \ldots, z_{r-1})$. There is in z-space a point where the system has r-pure phases, lines with $r-1$ phases, two dimensional surfaces with $r-2$ phases, etc.

1. Introduction

In this article we analyze the structure of Gibbs states, i.e. the phase diagram, for r-component non-symmetric continuum Widom-Rowlinson models at large fugacities. The notions of Gibbs states were introduced by Dobrushin [4, 5] and Lanford-Ruelle [7] as random fields with specified conditional probability distributions to describe the equilibrium states of the system.

The rigorous proof for the coexistence of Gibbs states for two-component symmetric continuum Widom-Rowlinson models was given by Ruelle [16], see also [8], by a (non-trivial) generalization of the Peierls argument for lattice systems. His argument can be extended to r-component models in which the different components are identical except for labeling. The coexistence of r-phases occurs when all fugacities are *equal* and large enough. Cassandro and Da Fano [2] obtained the asymptotic properties for correlation functions of contours for the symmetric Widom-Rowlinson model. They used the method

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of integral equations for the chain correlation functions, first proposed by Minlos and Sinai [11, 12] for the Ising model.

The symmetry requirement is built into these argument in a way which seems very hard to relax. In particular they require a priori knowledge of the parameter values at which the phase transition will occur, e.g. equal fugacities. This makes it hard to see how the Ruelle method can be generalized to cases where this information is not known in advance, i.e. for the ordinary liquid-vapour transition in a one component system. In fact it is difficult to see how the Peierls method can ever lead to a proof of coexistence of phases which are not connected by symmetry. It is the purpose of this paper to make a start on overcoming this burden of symmetry.

Our method is based on generalizing the Pirogov-Sinai theory [13, 14, 17] of phase transitions at low temperatures in non-symmetric lattice systems. The basic idea of the Pirogov-Sinai theory is that, at least at low temperatures, the homogeneous pure phases are simply related to the, not necessarily symmetric, ground states of the Hamiltonian. In our model the ground states will correspond to the Gibbs states in the limit of equal infinite fugacities of all components. There are r such ground states each containing only one type of particles. Since the interactions are not required to be symmetric however, the coexistence of pure phases will occur at large unequal fugacities with each pure phase consisting primarily of one component.

The outline of the rest of this paper is as follows. In Sect. 2 we give a precise description of our model. We consider explicitly only the case where the particles move in two dimensional space but our results are valid also for all higher dimensions. We also introduce there the notion of contours, which are the Pirogov-Sinai excitations of the ground states. We use here Ruelle's basic construction for transcribing lattice notions into continuum systems. Section 3 states the results and Sects. 4 and 5 give the basic estimates on contour correlations and proofs. In cases where the arguments are similar to those of Pirogov-Sinai the proofs are only sketched. Section 6 gives some physical background and discusses further extensions of the results.

2. Description of Model and Definitions

2.1 *r-state Widom-Rowlinson Model*

We consider a system in the two-dimensional plane $\mathbb{R}^2$ consisting of r species of particles with fugacities z_α, $\alpha \in \mathcal{S} \equiv \{0, 1, \ldots, r-1\}$. The interaction between α and β-particles is via a hard core pair potential

$$\phi_{\alpha,\beta}(\mathrm{r}) = \begin{cases} \infty & \text{if } |\mathrm{r}| \leqq R_{\alpha,\beta} \\ 0 & \text{otherwise,} \end{cases} \tag{2.1}$$

$R_{\alpha,\beta} \geqq \varepsilon > 0$ for $\alpha \neq \beta$, $R_{\alpha,\alpha} = 0$.

Let V be a square in $\mathbb{R}^2$. We denote the configurations of particles in V by

$$\xi_V = (\underline{x}_0, \dots, \underline{x}_{r-1}),$$

where $\underline{x}_\alpha = (x_1^\alpha, \dots, x_{n_i}^\alpha) \in \overbrace{V \times \dots \times V}^{n_i}$ is the configuration of α-type particles.

When $\xi = (\underline{x}_0, \dots, \underline{x}_{r-1})$ is given, the distance between $\underline{x}_\alpha = (x_1^\alpha, \dots, x_{n_i}^\alpha)$ and $\underline{x}_\beta = (x_1^\beta, \dots, x_{n_j}^\beta)$ is defined by

$$d(\underline{x}_\alpha, \underline{x}_\beta) = \operatorname*{Min}_{k,l} |x_k^\alpha - x_l^\beta|.$$

The partition function for the system is given by

$$Z(V) = \sum_{n_0 \dots n_{r-1}} \frac{1}{n_0! \dots n_{r-1}!} z_0^{n_0} \cdot z_1^{n_1} \cdot \dots \cdot z_{r-1}^{n_{r-1}} \cdot \int_V d^{n_0} \underline{x}_0 \int_V d^{n_1} \underline{x}_1 \dots \int_V d^{n_{r-1}} \underline{x}_{r-1} \, W(\underline{x}_0, \dots, \underline{x}_{r-1}) \tag{2.2}$$

$$W(\underline{x}_0, \dots, \underline{x}_{r-1}) = \begin{cases} 0 & \text{if } d(\underline{x}_\alpha, \underline{x}_\beta) < R_{\alpha,\beta} \text{ for some } (\alpha, \beta) \\ 1 & \text{otherwise,} \end{cases}$$

where we used the notation

$$\int_V d^{n_i} \underline{x}_i = \int_{\underbrace{V \times V \times \dots \times V}_{n_i}} dx_1^i \, dx_2^i \dots dx_{n_i}^i.$$

2.2 Definition of Contours

Consider the configuration $\xi = (\underline{x}_0, \dots, \underline{x}_{r-1})$ in $\mathbb{R}^2$ satisfying

$$d(\underline{x}_\alpha, \underline{x}_\beta) > R_{\alpha,\beta} \quad \text{for all } \alpha \neq \beta. \tag{2.3}$$

We cover R^2 with a grid $(d \cdot \mathbb{Z}^2)$ of spacing d. The squares of this grid are called *elementary squares*. We choose d sufficiently small, so that two particles of different species cannot be found in the same or in adjacent squares, i.e. $d < \frac{1}{2\sqrt{2}} \operatorname*{Min}_{\alpha \neq \beta} R_{\alpha,\beta}$. (Two squares are adjacent if they touch by a side or a corner.) However, for simplicity of notation, we shall from now on redefine our unit of length $d = 1$. Also, if Λ is a set of elementary squares, $|\Lambda|$ denotes the number of elementary squares in Λ and $\bar{\Lambda} = R^2 \setminus \Lambda$, the complement of Λ.

To each elementary square t we assign a label $\alpha(t) \in \{0, 1, \dots, r\}$ as follows;

$$\alpha(t) = \begin{cases} r & \text{if there is no particle in } t \\ j & \text{if there is at least one particle of type } j \text{ in } t. \end{cases}$$

When $\alpha(t) = j$, we say that t is a j-square.

Take a square C_0 of side $(N-1)d > 2R$, $R = \operatorname*{Max}_{\alpha \neq \beta} R_{\alpha,\beta}$, and put

$$C_i = C_0 + i, \quad i \in Z^2.$$

For a given configuration ξ, a square C_i is called irregular if there are two elementary squares t_1 and t_2 in C_i with $\alpha(t_1)\neq\alpha(t_2)$ and $\alpha(t_1)\neq r$, $\alpha(t_2)\neq r$. Other squares are called regular. Thus, in a regular square, there is only one type of particles.

Let Γ denote a connected set of irregular squares. A *contour* $\mathit{\Pi}$ is a pair; Γ and the set $\alpha(\Gamma)=\{\alpha(t); t\in\Gamma\}$ of labels in Γ, $\mathit{\Pi}=(\Gamma,\alpha(\Gamma))$.

The complement of Γ, $\bar{\Gamma}$ is decomposed into connected components. There is one infinite component called $\mathrm{Ext}\,\mathit{\Pi}$ and several finite ones whose union is $\mathrm{Int}\,\Gamma$. We can associate, in a unambiguous way, a given type of particles to the boundary of each of these components. We decompose $\mathrm{Int}\,\mathit{\Pi}=\bigcup_{m\in\mathscr{S}}\mathrm{Int}_m\mathit{\Pi}$ according to this label and we denote by $o(\Gamma)$ the label associated with $\mathrm{Ext}\,\mathit{\Pi}$. Finally let $A_q=\{\Gamma; o(\mathit{\Pi})=q\}$ and $\theta(\mathit{\Pi})=\mathit{\Pi}\cup\mathrm{Int}\,\mathit{\Pi}$. We shall use later the following obvious observation; there is a constant $k_1'>0$ (at least $3/N^2$) such that

$$\#\{t\in\Gamma; \alpha(t)=r\}>k_1'\,|\Gamma|.$$

Let $\mathscr{F}$ denote the totality of contours which are obtained from all configurations and let $\partial=\{\mathit{\Pi}_1,\dots,\mathit{\Pi}_s\}$ be the set of contours which is obtained from some particular configuration.

For a given ∂, there will be only one type of particles which can be put into any square $t\in V\setminus\bigcup_{i=1}^{s}\Gamma_i$. We associate the corresponding label to each such square. With such a labeling $V\setminus\bigcup_{i=1}^{s}\Gamma_i$ is decomposed into r components according to the label, $m\in\mathscr{S}$.

We denote the m component by $V_m(\partial)$. Given a set of contours, we distinguish the *outer contours* those that are not contained in the interior of any other contour. Finally we observe that, in the complement of the set of contours, the system is a free gas, with one species of particles in any connected set and with no influence from the other species.

2.3 *Definition of Gibbs Measure*

Let $\mathscr{M}$ be the set of all families $\partial=\{\mathit{\Pi}_i\}_{i\in I}$ of contours in R^2. We say that the family of contours $\partial=(\mathit{\Pi}_1,\dots,\mathit{\Pi}_s)$ is compatible with (V,q) if the following conditions i)–v) are satisfied:

i) $\mathit{\Pi}_i\in\mathscr{F}$ for each $\mathit{\Pi}_i$

ii) $O(\Gamma)=q$ for each outer contour $\mathit{\Pi}$ of ∂

iii) $d(\Gamma,\bar{V})\geqq 1$ for each $\mathit{\Pi}$ of ∂

iv) there is no contradiction in boundary conditions of ∂

v) $d(\Gamma_i,\Gamma_j)>1$ for each $i\neq j$.

We denote by $\mathscr{M}_{V,q}$ the totality of the family of contours which is compatible with (V,q).

For each $\mathit{\Pi}=(\Gamma,\alpha(\Gamma))$ we denote by $\{s_1,\dots,s_k\}\subset\Gamma$ the set of elementary squares $s_i\subset\Gamma$ such that $\alpha(s_i)\neq r$. We define the functional $\tilde{Z}(\mathit{\Pi})$ of Γ by

$$\tilde{Z}(\Pi)=\sum_{n_1=1}^{\infty}\cdots\sum_{n_k=1}^{\infty}\frac{z^{n_1}_{\alpha(s_1)}\cdots z^{n_k}_{\alpha(s_k)}}{n_1!\ldots n_k!}\int_{s_1}\cdots\int_{s_k} d^{n_1}x^{s_1}_{\alpha(s_1)}\ldots d^{n_k}x^{s_k}_{\alpha(s_k)}\,W(\underline{x}^{s_1}_{\alpha(s_1)},\ldots,\underline{x}^{s_k}_{\alpha(s_k)}),$$

where $\underline{x}^{s_i}_{\alpha(s_i)}$ is the configuration of particles of type $\alpha(s_i)$ in the elementary square s_i.

The Gibbs measure $P_{V,q}(\cdot)$ in V with q-boundary condition is given by

$$P_{V,q}(\partial)=\chi_{V,q}(\partial)\frac{1}{Z^q(V)}\prod_{\Pi\in\partial}\tilde{Z}(\Pi)\prod_{m\in\mathscr{S}}Z^m_f(V_m(\partial)),\tag{2.5}$$

where

$$\chi_{V,q}(\partial)=\begin{cases}1 & \text{if } \partial\in\mathscr{M}_{V,q}\\ 0 & \text{otherwise,}\end{cases}$$

$Z^m_f(V_m(\partial))=\exp\{z_m|V_m(\partial)|\}$ is the partition function of a free gas of m-type in $V_m(\partial)$, and $Z^q(V)$ is the normalization constant.

We next define the Gibbs measure of outer contours. Let

$$\mathscr{M}^{\text{out}}_{V,q}=\{\partial=(\Pi_1\ldots\Pi_s)\in\mathscr{M}_{V,q}:\theta(\Pi_i)\cap\theta(\Pi_j)=\phi(i\neq j)\}.$$

The Gibbs measure $P^{\text{out}}_{V,q}(\cdot)$ of outer contours is defined by

$$\begin{aligned}P^{\text{out}}_{V,q}(\partial)&=\chi^{\text{out}}_{V,q}(\partial)\frac{1}{Z^q(V)}Z^q_f(V\setminus\bigcup_{\Pi\in\partial}\theta(\Pi))\prod_{\Pi\in\partial}\tilde{Z}(\Pi)\prod_{m}Z^m(\text{Int}_m\Gamma)\\&=\chi^{\text{out}}_{V,q}(\partial)\frac{Z^q_f(V)}{Z^q(V)}\prod_{\Pi\in\partial}\frac{\tilde{Z}(\Pi)}{Z^q_f(\Pi)}\prod_{m}\frac{Z^m(\text{Int}_m\Gamma)}{Z^q_f(\text{Int}_m\Gamma)},\end{aligned}\tag{2.6}$$

where

$$\chi^{\text{out}}_{V,q}(\partial)=\begin{cases}1 & \text{if } \partial\in\mathscr{M}^{\text{out}}_{V,q}\\ 0 & \text{otherwise.}\end{cases}$$

3. Statement of Results

Throughout this section we fix the fugacity z_0 sufficiently large, put $\hat{z}=(z_1\ldots z_{r-1})\in\mathbb{R}^{r-1}$ and consider the parameter space

$$U(\varepsilon_0;z_0)=\{\hat{z}\in\mathbb{R}^{r-1};|\hat{z}-\hat{z}(0)|\equiv\max_{1\leq i\leq r-1}|z_i-z_i(0)|<\varepsilon_0 z_0\},$$

where $\hat{z}(0)=(z_0,z_0,\ldots,z_0)$.

We define the correlations functions of outer contours by

$$\rho^{\hat{z}}_{V,q}(\partial)=\sum_{\partial'\supset\partial}P^{\text{out}}_{V,q}(\partial').$$

Estimates for the correlation functions of outer contours play an important role in the proof of the phase-coexistence. In particular consider the estimates

$$\rho^{\hat{z}}_{V,q}(\partial)\leqq\exp\{-\tfrac{1}{2}z_0|\partial|\},\tag{3.1}$$

$$|\rho^{\hat{z}}_{V,q}(\Pi_1, \Pi_2) - \rho^{\hat{z}}_{V,q}(\Pi_1)\rho^{\hat{z}}_{V,q}(\Pi_2)| \leqq \exp\{-\tfrac{1}{2}z_0(|\Pi_1|+|\Pi_2|) - c\,z_0 d(\Pi_1, \Pi_2)\}, \tag{3.2}$$

where $c>0$ is a constant and $d(\Pi_1, \Pi_2)$ is the distance between Π_1 and Π_2. If these estimates are satisfied for k-different boundary conditions q then there are (at least) k-pure phases [17].

Theorem. *For sufficiently large $z_0>0$ and some $\varepsilon_0>0$, we have the following picture:*

I) *There exists a point $\hat{z}_0 \in \mathscr{U}(\varepsilon_0; z_0)$ such that the estimates* (3.1) *and* (3.2) *are satisfied for all $q\in\mathscr{S}$ when $\hat{z}=\hat{z}_0$,*

II) *There exist curves $\gamma_0, \gamma_1, \ldots, \gamma_{r-1} \subset \mathscr{U}(\varepsilon_0; z_0)$ each of which starts from $\hat{z}_0$ and* (3.1) *and* (3.2) *are satisfied for any $q\in\mathscr{S}\setminus\{\alpha\}$ when $\hat{z}\in\gamma_\alpha$.*

III) *There exist 2-dimensional open surfaces $\gamma_{\alpha,\beta} \subset \mathscr{U}(\varepsilon_0; z_0)$, $\alpha, \beta \in \mathscr{S}$, the boundary of which is given by $\bar{\gamma}_\alpha$ and $\bar{\gamma}_\beta$, and* (3.1) *and* (3.2) *are satisfied for any $q\in\mathscr{S}\setminus\{\alpha,\beta\}$ when $\hat{z}\in\gamma_{\alpha,\beta}$.*

IV) *In general, there exist k-dimensional open surfaces $\gamma_A \subset \mathscr{U}(\varepsilon_0; z_0)$, $A\subset\mathscr{S}$ and $\# A = k$, the boundary of γ_A is given by $\bar{\gamma}_{A\setminus\{\alpha\}}$, $\alpha\in A$, and* (3.1) *and* (3.2) *are satisfied for any $q\in\mathscr{S}\setminus A$ when $\hat{z}\in\gamma_A$.*

Furthermore $\bigcup_{A\subset\mathscr{S}} \bar{\gamma}_A \supset \mathscr{U}(\varepsilon_0; z_0)$, where $\bar{\gamma}_A$ is the closure of γ_A.

Let us remark that if follows from (3.1) that the probability

$$P^{\hat{z}}_{V,q}(\xi\in\mathscr{M}_{V,q};\ \text{the square at 0 is a } q\text{-square under } \xi) \geqq 1 - g(z_0) \tag{3.3}$$

uniformly in V, where $g(z_0)\to 0$ as $z_0\to\infty$. This estimate means that typical configurations in V with q-boundary conditions consist of a large "sea" of q-squares with small "islands" of other types of squares, surrounded by contours. In other words, for value of $\hat{z}$ in γ_A, the limiting Gibbs measures $\{P^{\hat{z}}_q(\cdot)\}_{q\in\mathscr{S}\setminus A}$ obtained from $P^{\hat{z}}_{V,q}$ by taking the limit $|V|\to\infty$ are all distinct. Furthermore each limiting Gibbs measure $P^{\hat{z}}_q(\cdot)$ satisfies the estimate (3.2) and hence is indecomposable, i.e. it represents a pure phase.

Thus we have the Pirogov-Sinai picture of the phase diagram [13, 14, 17]: r phases coexist when $\hat{z}=\hat{z}_0$, $r-1$ phases except the α-phase coexist when $\hat{z}\in\gamma_\alpha$, etc.

4. Contour Model

In this section we introduce the contour model and summarize the properties of correlation functions of contours without giving detailed proofs. The proofs are similar to those in the Pirogov-Sinai papers [13, 14] and in Chap. 2 of [17], to which we refer for details.

4.1 Rarefied Partition Function and Crystalline Partition Function

Let us consider the configurations in which $\Pi\in A_q$ is the only contour. The probability of such configuration is given by

$$P_{V,q}(I\Gamma)=\frac{1}{Z^q(V)}\tilde{Z}(I\Gamma)\cdot Z_f^q(V\setminus 0(I\Gamma))\prod_m Z_f^m(\mathrm{Int}_m I\Gamma)$$
$$=\frac{Z_f^q(V)}{Z^q(V)}\frac{\tilde{Z}(I\Gamma)}{Z_f^q(I\Gamma)}\prod_m\frac{Z_f^m(\mathrm{Int}_m)}{Z_f^q(\mathrm{Int}_m)}$$
$$=\frac{1}{Z_0^q(V)}\frac{\tilde{Z}(I\Gamma)}{Z_f^q(I\Gamma)}\prod_m \exp\{(z_m-z_q)|\mathrm{Int}_m\Gamma|\} \tag{4.1}$$

where $Z_0^q(V)=Z^q(V)/Z_f^q(V)$.

Setting

$$H_q^{\hat{z}}(I\Gamma)=-\log\left(\frac{\tilde{Z}(I\Gamma)}{Z_f^q(I\Gamma)}\prod_m \exp\{(z_m-z_q)|\mathrm{Int}_m\Gamma|\}\right), \tag{4.2}$$

we then have

$$P_{V,q}(I\Gamma)=\frac{1}{Z_0^q(V)}\exp\{-H_q^{\hat{z}}(I\Gamma)\}. \tag{4.3}$$

It follows from the definition of contour that there exists a constant k_1', $0<k_1'<1$ satisfying

$$\#\{t\in\Gamma:\alpha(t)=r\}>k_1'|\Gamma|$$

for each $I\Gamma$, so that we have

$$\hat{Z}(I\Gamma)\leqq\exp\{k_1 z_0|I\Gamma|\} \tag{4.4}$$

for some constant $k_1<1$ if $\hat{z}=\hat{z}(0)$.

Hence, $H_q^{\hat{z}}(I\Gamma)$ has a lower bound proportional to $|I\Gamma|$ if $\hat{z}=\hat{z}(0)$, i.e. it satisfies the Peierls condition, see [17]

$$H_q^{\hat{z}}(I\Gamma)\geqq k_2 z_0|I\Gamma|,$$

where $k_2>0$ is a constant.

Let us consider the configurations in which $I\Gamma$ is the only outer contour. The probability of such configurations is given by

$$P_{V,q}^{\mathrm{out}}(I\Gamma)=\frac{1}{Z^q(V)}Z_f^q(V\setminus 0(I\Gamma))\cdot\tilde{Z}(I\Gamma)\prod_m Z^m(\mathrm{Int}_m I\Gamma)$$
$$=\frac{1}{Z_0^q(V)}\frac{\tilde{Z}(I\Gamma)}{Z_f^q(I\Gamma)}\prod_m\frac{Z^m(\mathrm{Int}_m I\Gamma)}{Z_f^q(\mathrm{Int}_m I\Gamma)}. \tag{4.5}$$

If we put

$$Z_0^q(I\Gamma)=\frac{\tilde{Z}(I\Gamma)}{Z_f^q(I\Gamma)}\prod_m\frac{Z^m(\mathrm{Int}_m I\Gamma)}{Z_f^q(\mathrm{Int}_m I\Gamma)}, \tag{4.6}$$

then

$$P_{V,q}^{\mathrm{out}}(I\Gamma)=\frac{Z_0^q(I\Gamma)}{Z_0^q(V)}. \tag{4.7}$$

More generally

$$P_{V,q}^{\mathrm{out}}(I\Gamma_1,\dots,I\Gamma_s)=\frac{1}{Z_0^q(V)}\prod_{i=1}^{s}Z_0^q(I\Gamma_i). \tag{4.8}$$

We call $Z_0^q(V)$ and $Z_0^q(\Pi\Gamma)$ the rarefied partition functions and the crystalline partition functions respectively. We have the following relation between the rarefied partition function and the crystalline partition function; cf. Eqs. (2.17), (2.18) in [17]:

Lemma 4.1

i) $$Z_0^q(V) = \sum_{\{\Pi\Gamma_1, \ldots, \Pi\Gamma_s\}:\,\text{outer in } V} \prod_{i=1}^{s} Z_0^q(\Pi\Gamma_i) \tag{4.9}$$

ii) $$Z_0^q(\Pi\Gamma) = \exp\{-H_q^{\pm}(\Pi\Gamma)\} \prod_m Z_0^m(\mathrm{Int}_m \Pi\Gamma). \tag{4.10}$$

4.2 Contour Model

We now introduce the probability distribution on the set of families of contours with the same outer boundary conditions. This is called the contour model. Since all contours have the same outer boundary conditions, such families do not necessarily correspond to realizable configurations. But for such a simple system we can apply the usual Peierls argument and obtain the properties of correlation functions of contours in the same way as in the Ising model. In Sect. 5 we will give the precise relation between the contour and the real system.

We shall now define the contour model more exactly. We say that a family of contours $\partial = \{\Pi\Gamma_1, \ldots, \Pi\Gamma_k\}$ of A_q is compatible if $d(\Gamma_i, \Gamma_j) > 1$ for all $i \neq j$. Let D_q denote the totality of compatible families of contours. Consider the functional $F_q(\cdot)$ on A_q which satisfies

$$\sup_{\Pi\Gamma \in A_q} \frac{|F_q(\Pi\Gamma)|}{|\Pi\Gamma|} < \infty$$

and $F_q(\Pi\Gamma) \geqq \tau|\Pi\Gamma|$, $\tau > 0$.

We call such a functional $F_q(\cdot)$ τ-functional.

The contour model is the probability distribution on D_q defined by

$$P_{V,q}(\partial) = \chi_V(\partial) \cdot \frac{1}{Z(V|F_q)} e^{-F_q(\partial)}, \tag{4.11}$$

where

$$\chi_V(\partial) = \begin{cases} 1 & \text{if } \partial \subset V, \text{ for all } \Pi\Gamma \in \partial \\ 0 & \text{otherwise} \end{cases}$$

$$F_q(\partial) = \sum_{\Pi\Gamma \in \partial} F_q(\Pi\Gamma),$$

and $Z(V|F_q)$ is the normalisation constant.

We define the crystalline partition function $Z(\Pi\Gamma|F_q)$ for the contour model by

$$Z(\Pi\Gamma|F_q) = e^{-F_q(\Pi\Gamma)} \sum_{\partial \subset \mathrm{Int}\,\Pi\Gamma} e^{-F_q(\partial)}. \tag{4.12}$$

We have the following obvious relations between $Z(V|F_q)$ and $Z(\Pi\Gamma|F_q)$:

Lemma 4.2

i) $Z(V|F_q)=\sum_{\{\Pi\Gamma_1,\ldots,\Pi\Gamma_s\}:\text{outer in }V}\prod_{i=1}^{s} Z(\Pi\Gamma_i|F_q)$ (4.13)

ii) $Z(\Pi\Gamma|F_q)=e^{-F_q(\Pi\Gamma)}\prod_m Z(\mathrm{Int}_m\Pi\Gamma|F_q)$. (4.14)

For each $\partial\in D_q$ let $\Phi(\partial)$ denote the totality of outer contours. We define the correlation function of contours by

$$\lambda_V(\partial|F_q)=\sum_{\tilde\partial\supset\partial}P_{V,q}(\tilde\partial). \tag{4.15}$$

For each $\partial\in D_q$ satisfying $\partial\subset V$ and $\Phi(\partial)=\partial$, we define the correlation functions of outer contours by

$$\rho_V(\partial|F_q)=\sum_{\tilde\partial:\partial\subset\Phi(\tilde\partial)}P_{V,q}(\tilde\partial). \tag{4.16}$$

Since the outer conditions of all contours in ∂ are fixed to be q, the following estimate for correlation functions are easily obtained from the standard Peierls argument (see e.g. [17], Lemma 2.6 and Proposition 2.2).

Lemma 4.3 *(Peierls inequality)*

i) $\lambda_V(\partial|F_q)\leqq e^{-F_q(\partial)}$

ii) $\rho_V(\partial|F_q)\leqq e^{-F_q(\partial)}$.

In the same way as in the Ising model, we introduce the infinite volume contour correlation equations. These equations are expressed as equations in some appropriate Banach space. (See p. 52 of [17].) They have unique solutions $\lambda(\cdot|F_q)$ and $\rho(\cdot|F_q)$ whenever τ is sufficiently large. We summarize the properties of these correlation functions in the following.

Lemma 4.4 ([13, 14, 17]). *For sufficiently large τ the following properties are satisfied:*

1) $|\lambda_V(\partial|F_q)-\lambda(\partial|F_q)|<C_2e^{-\tau(|\partial|+d(\partial,V^c))}$ (4.17)

2) $|\rho_V(\partial|F_q)-\rho(\partial|F_q)|<C_2e^{-\tau(|\partial|+d(\partial,V^c))}$ (4.18)

3) $|\rho_V(\partial_1,\partial_2|F_q)-\rho_V(\partial_1|F_q)\rho_V(\partial_2|F_q)|<C_3e^{-\tau(|\partial_1|+|\partial_2|+d(\partial_1,\partial_2))}$ (4.19)

where $|\partial_i|=\sum_{\Pi\Gamma\in\partial_i}|\Pi\Gamma|$ *and* C_1, C_2, C_3 *are constants.*

Using the following obvious lemma, the proof of the above lemma is obtained in the same way as in [13, 14, 17].

Lemma 4.5. *There exists a constant $C_0>0$ such that*

$$\#\{\Pi\Gamma\in A_q;\ \theta(\Pi\Gamma)\ \textit{contains the origin and}\ |\Pi\Gamma|=k\}\leqq C_0^k.$$

By using the estimates for $\lambda_{V,q}(\cdot)$ and $\lambda(\cdot)$, we can prove the existence of the following limit (see [17], Proposition 2.3):

Lemma 4.6. *For sufficiently large τ, the limit*

$$S(F_q)=\lim_{|V|\to\infty}\frac{1}{|V|}\ln Z(V|F_q)$$

exists, and satisfies

$$|\Delta(V|F_q)| \leqq e^{-\tau}|\partial V|, \tag{4.20}$$

where

$$\Delta(V|F_q) = \ln Z(V|F_q) - S(F_q)|V|. \tag{4.21}$$

The limit $S(F_q)$ can be expressed in the form

$$S(F_q) = \int_1^{\tau} \sum_{\gamma} F(\gamma)\lambda(\gamma|F_q^t)\,dt,$$

where γ is a congruence class of contours and $\lambda_q(\gamma,t)$ is the infinite volume correlation function with respect to the functional $F_q^t(\cdot) \equiv t F_q(\cdot)$. From this formula we have $S(F_q) \leqq e^{-\tau}$.

By using the estimate (4.17), we can obtain (4.21).

Now we introduce the parametric partition function $Z(V;F_q,b)$ given by

$$Z(V;F_q,b) = \sum_{\partial:\Phi(\partial)=\partial\subset V} \prod_{\Pi\Gamma\in\partial} Z(\Pi\Gamma|F_q)e^{|\mathrm{Int}\,\Pi\Gamma|} \tag{4.22}$$

and put $\Delta(V|F_q,b) = \ln Z(V;F_q,b) - (S(F_q)+b)|V|$.

Then the following estimate follows directly from the definition,

$$-b|V| + e^{-\tau}|\partial V| \leqq \Delta(V|F_q,b) \leqq e^{-\tau}|\partial V|. \tag{4.23}$$

For each functional $F_q(\cdot)$ defined on A_q we define the norm $\|F_q\|$ by

$$\|F_q\| = \sup_{\Pi\Gamma\in A_q} \frac{F_q(\Pi\Gamma)}{|\theta(\Pi\Gamma)|\,C_0^{\delta(\Pi\Gamma)}},$$

where $\delta(\Pi\Gamma)$ is a diameter of $\Pi\Gamma$.

Lemma 4.7

i) $|S(F_q^1) - S(F_q^2)| \leqq e^{-C_1\tau}\|F_q^1 - F_q^2\|$ (4.24)

ii) $|\Delta(V|F_q^1,b^1) - \Delta(V|F_q^2,b^2)|$

$$\leqq 2|b^1-b^2||V| + \left(\frac{1}{C_0-1} + e^{-C_1\tau}\right) C_0^{\delta(V)}|V|\,\|F_q^1 - F_q^2\|, \tag{4.25}$$

where C_1 is a constant.

For a proof, see [17], Propositions 2.4 and 2.5.

5. Proof of Theorem

Proposition 5.1. 1) *For sufficiently large z_0, some $\varepsilon_0 > 0$, and each $\hat{z} \in \mathcal{U}(z_0;\varepsilon_0)$ there exists a unique family $\hat{F} = (F_0, F_1, \ldots, F_{r-1})$ of translation invariant τ-functionals with $\tau = c z_0$, $c > 0$ which satisfies*

$$Z_0^q(\Pi\Gamma) = \exp\{b_q|\mathrm{Int}\,\Pi\Gamma|\}\, Z(\Pi\Gamma|F_q) \tag{5.1}$$

for each $\Pi\Gamma \in A_q$, *where*

$$b_q = z_q - S(F_q) + \alpha \tag{5.2}$$

and α *is determined by* $\operatorname{Min} b_q = 0$.

2) *Furthermore* $\hat{F}$ *satisfies*

$$\|\hat{F}(\hat{z}^1) - \hat{F}(\hat{z}^2)\| < 8\,|\hat{z}^1 - \hat{z}^2|, \qquad \hat{z}^1, \hat{z}^2 \in \mathscr{U}(z_0; \varepsilon_0), \tag{5.3}$$

where $\|\hat{F}\| = \operatorname{Max}\{\|F_0\|, \|F_1\|, \ldots, \|F_{r-1}\|\}$.

Proof. For each $\hat{z} \in \mathscr{U}(z_0; \varepsilon_0)$, (5.1) is considered to be a system of equations for $\hat{F}$.

From (4.9) and (5.1) we obtain

$$Z_0^q(V) = Z(V\,|\,F_q, b_q). \tag{5.4}$$

Substituting (5.1) and (5.4) into (4.10) and taking the logarithm we obtain

$$b_q\,|\operatorname{Int}\Pi\Gamma| + \ln Z(\Pi\Gamma\,|\,F_q) = -H_q^{\pm}(\Pi\Gamma) + \sum_m \ln Z(\operatorname{Int}_m \Pi\Gamma\,|\,F_m, b_m). \tag{5.5}$$

We now decompose $\ln Z(\Pi\Gamma\,|\,F_q)$ and $\ln Z(\operatorname{Int}_m \Pi\Gamma\,|\,F_m, b_m)$ into the following forms:

$$\ln Z(\Pi\Gamma\,|\,F_q) = -F_q(\Pi\Gamma) + S(F_q)\,|\operatorname{Int}\Pi\Gamma| + \sum_m \Delta(\operatorname{Int}_m \Pi\Gamma\,|\,F_q)$$

$$\ln Z(\operatorname{Int}_m \Pi\Gamma\,|\,F_m, b_m) = (S(F_m) + b_m)\,|\operatorname{Int}_m \Pi\Gamma| + \Delta(\operatorname{Int}_m \Pi\Gamma\,|\,F_m, b_m). \tag{5.6}$$

Then, by substituting (5.6) into (5.5) and using (5.2) and (4.2), we find that

$$\begin{aligned} F_q(\Pi\Gamma) &= \sum_m \{(S(F_q) + b_q) - (S(F_m) + b_m)\}\,|\operatorname{Int}_m \Pi\Gamma| \\ &\quad + H_q^{\pm}(\Pi\Gamma) + \sum_m \{\Delta(\operatorname{Int}_m \Pi\Gamma\,|\,F_q) - \Delta(\operatorname{Int}_m \Pi\Gamma\,|\,F_m, b_m)\} \\ &= \{z_q\,|\Gamma| - \ln \check{Z}(\Pi\Gamma)\} + \sum_m \{\Delta(\operatorname{Int}_m \Pi\Gamma\,|\,F_q) - \Delta(\operatorname{Int}_m \Pi\Gamma\,|\,F_m, b_m)\} \end{aligned} \tag{5.7}$$

holds for each $\Pi\Gamma \in A_q$ and $q = 0, 1, \ldots, r-1$.

We rewrite (5.7) in the following form

$$F_q(\Pi\Gamma) = J_q(\Pi\Gamma : \hat{z}) + T_q(\Pi\Gamma : \hat{F}, \hat{z}) \tag{5.7'}$$

where

$$J_q(\Pi\Gamma : \hat{z}) = z_q\,|\Gamma| - \ln \check{Z}(\Pi\Gamma)$$

$$T_q(\Pi\Gamma : F, \hat{z}) = \sum_m \{\Delta(\operatorname{Int}_m \Pi\Gamma\,|\,F_q) - \Delta(\operatorname{Int}_m \Pi\Gamma\,|\,F_m, b_m)\}. \tag{5.8}$$

Putting

$$\hat{T} = (T_0, T_1, \ldots, T_{r-1})$$

$$\hat{J} = (J_0, J_1, \ldots, J_{r-1}),$$

we have the equivalent form of (5.7),

$$\hat{F} = \hat{J}(\hat{z}) + \hat{T}(\hat{F}, \hat{z}). \tag{5.9}$$

It follows from (4.20) and (4.23) that

$$T_q(\mathbb{\Gamma}:\hat{F},\hat{z}) \geqq -2e^{-\tau}\sum_m |\hat{c}(\mathrm{Int}_m \mathbb{\Gamma})| \geqq -2e^{-\tau}|\mathbb{\Gamma}|.$$

Then we have the following inequality:

$$\begin{aligned}(\text{the r.h.s. of (5.7')}) &> z_q|\Gamma| - k_1(1+\varepsilon_0)z_0|\Gamma| - 2e^{-\tau}|\Gamma| \\ &> \tfrac{1}{2}(1-k_1)z_0|\Gamma| - 2e^{-\tau}|\Gamma|.\end{aligned}$$

For sufficiently small $\varepsilon_0 > 0$, this shows that the r.h.s. of (5.7') is a τ-functional with $\tau = \frac{1}{3}(1-k_1)z_0$ for sufficiently large z_0. We take $c = \frac{1}{3}(1-k_1)$.

The proof for the existence of the unique solution of (5.7') follows from the contraction property of $\hat{T}$,

$$\|\hat{T}(\hat{F}^1,\hat{z}) - \hat{T}(\hat{F}^2,\hat{z})\| < \tfrac{1}{2}\|\hat{F}^1 - \hat{F}^2\|. \tag{5.10}$$

We shall now prove (5.10). From Lemma 4.7 we obtain,

$$\begin{aligned}&|T_q(\mathbb{\Gamma}:\hat{F}^1,\hat{z}^1) - T_q(\mathbb{\Gamma}:\hat{F}^2,\hat{z}^2)| \\ &\quad\leqq \sum_m |\Delta(\mathrm{Int}_m \mathbb{\Gamma}|F_q^1) - \Delta(\mathrm{Int}_m \mathbb{\Gamma}|F_q^2)| + \sum_m |\Delta(\mathrm{Int}_m \mathbb{\Gamma}|F_m^1, b_m^1) - \Delta(\mathrm{Int}_m \mathbb{\Gamma}|F_m^2, b_m^2)| \\ &\quad\leqq 2|\hat{z}^1 - \hat{z}^2||\mathrm{Int}\,\mathbb{\Gamma}| + 2e^{-\tau}\cdot|\mathrm{Int}\,\mathbb{\Gamma}|\cdot\|F_q^1 - F_q^2\| \\ &\qquad + 2\left(\frac{1}{C_0 - 1} + e^{-\tau}\right)\cdot C_0^{\delta(\mathrm{Int}\,\mathbb{\Gamma})}\cdot|\mathrm{Int}\,\mathbb{\Gamma}|\cdot\|F_q^1 - F_q^2\|.\end{aligned}$$

This means

$$\|\hat{T}(\hat{F}^1,\hat{z}^1) - \hat{T}(\hat{F}^2,\hat{z}^2)\| < 2|\hat{z}^1 - \hat{z}^2| + \tfrac{1}{2}\|\hat{F}^1 - \hat{F}^2\|. \tag{5.11}$$

Choosing $\hat{z}^1 = \hat{z}^2$, we obtain the contraction property (5.10). We therefore have a unique solution $\hat{F} = \hat{F}(\hat{z})$ of (5.7') for each $\hat{z} \in \mathscr{U}(\varepsilon_0; z_0)$ and sufficiently large z_0.

Before proving the second assertion of Prop. 5.1, we state one more lemma.

Lemma 5.2. *If $z_m^1 \geqq 1$ and $z_m^2 \geqq 1$ for all m, then we have*

$$|\ln \tilde{Z}(\mathbb{\Gamma}:\hat{z}^1) - \ln \tilde{Z}(\mathbb{\Gamma}:\hat{z}^2)| \leqq 2|\mathbb{\Gamma}||\hat{z}^1 - \hat{z}^2|. \tag{5.12}$$

Proof of the Lemma. From the definition of $\tilde{Z}(\mathbb{\Gamma})$ we have

$$z_m \frac{\partial \ln \tilde{Z}(\mathbb{\Gamma}:\hat{z})}{\partial z_m} = E[\#\text{ of particles of type } m \text{ in } \mathbb{\Gamma}|\mathbb{\Gamma}].$$

Here $E[f|\mathbb{\Gamma}]$ is the expectation of the function f defined on the configuration space in $\mathbb{\Gamma}$ under the condition that the contour $\mathbb{\Gamma}$ exists, i.e.

$$\begin{aligned}E[f|\mathbb{\Gamma}] = \frac{1}{\tilde{Z}(\mathbb{\Gamma}:\hat{z})}\sum_{n_1=1}^{\prime}\cdots\sum_{n_k=1}^{\prime}\frac{z_{\alpha(s_1)}^{n_1}\cdots z_{\alpha(s_k)}^{n_k}}{n_1!\dots n_k!} \\ \cdot\int_{s_1}\cdots\int_{s_k} d^{n_1}\underline{x}_{\alpha(s_1)}\cdots d^{n_k}\underline{x}_{\alpha(s_k)} f(\underline{x}_{\alpha(s_1)}^{s_1}\cdots\underline{x}_{\alpha(s_k)}^{s_k})\cdot W(\underline{x}_{\alpha(s_1)}^{s_1},\dots,\underline{x}_{\alpha(s_k)}^{s_k}),\end{aligned}$$

where $\{s_1,\dots,s_k\} = \{t \in \mathbb{\Gamma}: \alpha(t) \neq r\}$.

For a given configuration $\underline{y}$ of particles in $\{t\in\Pi: \alpha(t)\neq m, r\}$ we define the probability density $p(\underline{y})$ by

$$p(\underline{y})=\frac{1}{\hat{Z}(\Pi:\hat{z})}\sum_{q_1=1}^{\infty}\cdots\sum_{q_p=1}^{\infty}\frac{z_m^{q_1+\cdots+q_p}}{q_1!\cdots q_p!}\cdot\int_{t_1}\cdots\int_{t_p}d^{q_1}\underline{x}_m^{t_1}\cdots d^{q_p}\underline{x}_m^{t_p}\cdot W(\underline{y},\underline{x}_m^{t_1},\ldots,\underline{x}_m^{t_p})$$

and define the conditional expectation $E[\cdot|\underline{y}]$ similarly to $E[\cdot|\Pi]$.

Then we obtain

$$\begin{aligned}&E[\#\text{ of particles of type } m \text{ in } \Pi|\Pi]\\&\quad=\int d\underline{y}\,p(\underline{y})E[\#\text{ of particle of type } m \text{ in } \Pi|\underline{y}].\end{aligned}$$

Let $N(W)$ denote the number of particles in W, and $\Pi(\underline{y}:m)$ denote the subregion of $\Pi(m)\equiv\{t\in\Gamma:\alpha(t)=m\}$ in which we can put m-type particles without interference from the configuration $\underline{y}$.

Putting $t(\underline{y})=t\cap\Pi(\underline{y}:m)$ for each square $t\in\Pi(m)$, and using standard probabilistic arguments we have

$$\begin{aligned}E[N(\Pi(m))|\underline{y}]&=\sum_{t\in\Pi(m)}\frac{z_m\cdot|t(\underline{y})|\,e^{z_m|t(\underline{y})|}}{e^{z_m|t(\underline{y})|}-1}\\&\leqq 2z_m\cdot|\Pi|.\end{aligned}$$

Hence we have

$$\frac{\partial\ln\hat{Z}(\Pi:\hat{z})}{\partial z_m}\leqq 2|\Pi|.$$

The proof of Lemma 5.2 follows directly from this estimate. □

Proof of Prop. 5.1, part 2:

From (5.7) and (5.12) we obtain

$$\|F_q(\hat{z}^1)-F_q(\hat{z}^2)\|<4|\hat{z}^1-\hat{z}^2|+\tfrac{1}{2}\|F_q(\hat{z}^1)-F_q(\hat{z}^2)\|.$$

Therefore, we obtain the second assertion of Prop. 5.1,

$$\|F_q(\hat{z}^1)-F_q(\hat{z}^2)\|<8|\hat{z}^1-\hat{z}^2|.\quad\square$$

Now we are in a position to prove the theorem.

Proof of Theorem. From Prop. 5.1 there exists the τ-functionals $\{F_q(\hat{z})\}_q$ with $\tau=\frac{1}{2}cz_0$ for each $\hat{z}\in\mathscr{U}(\varepsilon_0:z_0)$ satisfying

$$\begin{aligned}Z_0^q(\Pi)&=\exp\{b_q|\operatorname{Int}\Pi|\}\,Z(\Pi|F_q)\\b_q&=-z_q-S(F_q(\hat{z}))+\alpha.\end{aligned}\tag{5.14}$$

For a given $\hat{z}\in\mathscr{U}(\varepsilon_0:z_0)$ $b=(b_0,\ldots,b_{r-1})\in O_r$ is determined through $\hat{F}(\hat{z})$, where

$$O_r=\{b=(b_0,b_1,\ldots,b_{r-1}):\ \min_{0\geq k\geq r-1}b_k=0\}.$$

Let I_{z_0} denote the mapping from $\hat{z}\in\mathscr{U}(\varepsilon_0:z_0)$ to $b\in O_r$. We shall prove that I_{z_0} is a one-to-one continuous mapping and that $I_{z_0}\mathscr{U}(\varepsilon_0:z_0)\supset A$, where $A=\{b\in O_r:|b|<\frac{1}{3}\varepsilon_0 z_0\}$.

It follows from (4.24) and (5.3) that

$$\begin{aligned} |I_{z_0}(\hat z^1)-I_{z_0}(\hat z^2)| &< 2|\hat z^1-\hat z^2| + \max_{0\leq k\leq r-1} |S(F_k(\hat z^1))-S(F_k(\hat z^2))| \\ &< 2|\hat z^1-\hat z^2| + e^{-c_1 z_0}\ \hat F(\hat z^1)-\hat F(\hat z^2) \\ &< 2|\hat z^1-\hat z^2| + 8e^{-c_1' z_0}|\hat z^1-\hat z^2| \\ &< 3|\hat z^1-\hat z^2|. \end{aligned} \tag{5.15}$$

for sufficiently large z_0, with $c_1' = c_1 c$.

The continuity of I_{z_0} follows from (5.15).

When $b\in A$ is given

$$z_q = -(b_q + S(F_q(\hat z))) + \alpha, \qquad q\in\{0, 1, \ldots, r-1\} \tag{5.16}$$

can be considered as a system of equations for finding $\hat z$. From (5.16) we have

$$\begin{aligned} |z_q - z_0| &\leqq |b_q - b_0| + |S(F_0(\hat z)) - S(F_q(\hat z))| \\ &\leqq \tfrac{2}{3}\varepsilon_0 z_0 + 2e^{-cz_0} \end{aligned}$$

because $S(F_q) < e^{-cz_0}$.

Hence we have

$$|z_q - z_0| < \varepsilon_0 z_0 \tag{5.17}$$

for sufficiently large z_0.

Furthermore we have

$$|S(F_q(\hat z^1)) - S(F_q(\hat z^2))| \leqq 8e^{-cz_0}|\hat z^1 - \hat z^2|. \tag{5.18}$$

This means that the right hand side of (5.16) is a contraction for sufficiently large z_0.

We have thus proved that I_{z_0} is a one-to-one continuous mapping satisfying $I_{z_0}\mathscr{U}(\varepsilon_0, z_0)\supset A$ for sufficiently large z_0.

Put $\hat z_0 = I_{z_0}^{-1}(0)\in\mathscr{U}(\varepsilon_0 ; z_0)$ for sufficiently large z_0, then we have

$$Z_0^q(\Pi) = Z(\Pi|F_q) \quad \text{and} \quad Z_0^q(V) = Z(V|F_q) \tag{5.19}$$

for each $q\in\{0, 1, \ldots, r-1\}$. This means that

$$\rho_{V,q}(\hat c) = \rho_{V,q}(\hat c|F_q). \tag{5.20}$$

Then from Lemma 4.3 and 4.4 we have the first assertions of the theorem.

In general, by putting $\gamma_A = I_{z_0}^{-1}(E_A)$,

$$E_A = \{b\in O_r : b_i = 0\ i\in\mathscr{S}\setminus A\}, \qquad A\subset\mathscr{S},$$

we can prove the assertion of the theorem. Q.E.D.

6. Concluding Remarks

1. While the model discussed in this paper is certainly very idealized the structure of its phase diagram is similar to that of real multi-component

systems at fixed reciprocal temperature β. There too the thermodynamic parameter space is split into maximally connected sets characterized by the property that the number of coexisting pure phases is constant on each of them. It is this decomposition which is represented by the phase diagram of a macroscopic system [17].

The simplest such diagram is that of a one component system where the thermodynamic space has only two dimensions conveniently labelled by reciprocal temperature β and fugacity z. For most values of β and z the system is in some definite phase uniquely determined by the parameters, i.e. there is only one Gibbs state. There are, however, some values of β and z lying on smooth curves, at which the state of the system is *not unique* – it can exist in either of two pure states, a gas or a liquid, or a gas or a solid. At the triple point the system *can* exist in three different pure states – gas, liquid and solid. These states have different particle and energy densities, and one of them, the solid, even has a different symmetry. There may be other coexistence lines where the symmetry of the crystal changes or where quantum mechanically driven transitions occur. For a multi-component system the structure of the phase diagram is still richer. The thermodynamic parameter space now consists of β and all the fugacities z_i, $i=0,1,\ldots,r-1$, where r is the number of components. At fixed β the r-dimensional space with coordinates z_i split in the way we have seen it do for the Widom-Rowlinson model.

When the systems parameters move across a coexistence line or surface some properties of the system, e.g. density, composition, change discontinuously from their values in one of the pure phases to their values in the other. The system is then said to undergo a first order phase transition. The understanding of such transitions from first principles is the central theme of equilibrium statistical mechanics – a subject whose aim is the derivation of laws governing the equilibrium behavior of macroscopic objects from the laws governing the interaction of their microscopic constituents.

The first recorded theoretical speculations about the microscopic basis of phase transitions go back to ancient times – they are summarized in Lucretius' famous poetic review article De Rerum Natura [10]. The subject was taken up again in more recent times by van der Waals [18] and Gibbs [6]: the first constructing explicit, albeit approximate, formulae describing the liquid-gas transition and the latter creating a general macroscopic and microscopic formalism for dealing with this problem.

The key feature of the macroscopic or thermodynamic part of Gibbs' formalism is to consider the (appropriate) free energy of a macroscopic system as a function of the systems thermodynamic parameters. This function is convex and appropriate partial derivatives of it determine the density, concentration, etc. First order phase transitions then correspond to discontinuities in these derivatives. The microscopic part of Gibbs' formalism – our statistical mechanics – supplies a prescription for computing the free energy of a system with a given microscopic Hamiltonian.

Gibbs theory also provides us with ensembles, i.e. a probability distributions on the microscopic phase space of the system. All properties of a microscopic system (not just density, composition, energy) can be obtained as ensemble averages of suitable functions of the microscopic state of the system. We are particularly interested in the Gibbs state of the infinite volume, thermodynamic, limit of a physical system. As is well known it is this limit which properly represents bulk properties of a macroscopic system. Furthermore we are interested in systems with translation invariant interactions and therefore define pure phases to be translation invariant or periodic extremal Gibbs states [17, 15]. The existence of multiple pure phases is therefore connected with the non-uniqueness of the infinite volume limit which is what we have studied here.

2. The two component symmetric system of A and B particles with interactions (2.1) was introduced by Widom and Rowlinson [19] primarily for the purpose of gaining information about the liquid-vapour phase transition in a one component fluid. They noted that by integrating out the coordinates of one of the components, say the B ones, the probability measure on the A's in V is a Gibbs' measure for a one component system with many body interaction which could be written down explicitly. The phase transition in the A–B system when $z_A = z_B$ is large, whose existence they assumed on physical grounds, then translated into a liquid vapour transition in the A-system. The symmetry between the A-rich and B-rich pure phases on the coexistence line gave information about the corresponding liquid and vapour densities.

Ruelle [16] proved rigorously the existence of a phase transition in this model. His method could also treat the case where there were also hard core interactions between the A–A and B–B particles, $0 \leqq R_{AA} = R_{BB} < (1/5) R_{AB}$. As already mentioned in the introduction the A–B symmetry is crucial to Ruelle's method. This assures that the phase transition will occur for $z_A = z_B$. The method generalizes easily to an r-component system as long as $R_{\alpha\alpha} = R' \leqq CR_{\alpha\beta} = CR$, the same for all α and β, with $C < 1$ a suitable constant which depends on r. Clearly for this system the phase diagram will be symmetric; when $z_0 = z_1 = \ldots = z_{r-1} = \bar{z}$ sufficiently large there will be r pure phases, when $z_0 = \ldots = z_{i-1} = z_i = \ldots = z_{r-1} > z_i$ there will be $r-1$ phases, etc. Just how large $\bar{z}$ has to be depends on r (for fixed R). The proof requires $\bar{z} = O(\ln r)$ which also seems physically right – since the mixing entropy goes like $\ln r$.

The symmetric two component Widom-Rowlinson model is in many ways analogous to the ferromagnetic Ising lattice system. Many inequalities, such as FKG can be proven for this system, at least when $R_{\alpha\alpha} = 0$ [9]. These can be used to prove results about the existence and uniqueness of correlation functions when the infinite volume Gibbs states obtained as limits of finite volume states with A or B boundary conditions coincide [3].

In the present note we generalized Ruelle's result to the case where the $R_{\alpha\beta}$ are not equal. We did assume however that the $R_{\alpha\alpha}$ are all equal to zero. We do not know at the present time whether we can extend our results to the case $R_{\alpha\alpha} \neq 0$ for at least some α. The difficulty here lies in the fact that for the Pirogov-Sinai argument for the non-symmetric case we need some information about the behavior of the free energy and correlations in the one component system. This is trivial for $R_{\alpha\alpha} = 0$ when the one-component systems are free gases but not otherwise.

3. The analysis of this paper can be extended in a natural way to a model system of hard non-spherical molecules with a finite number of orientations, e.g. ellipsoids. In $\mathbb{R}^2$ we can consider the simple system consisting of "needles" of length b and zero width. Letting the needles take orientations specified by the angles $\theta_0, \theta_1, \ldots, \theta_{n-1}$, $0 \leqq \theta_\alpha \leqq \pi$ measured relative to the positive x-axis, we can identify each orientation as a different species $\theta_\alpha \Leftrightarrow \alpha \in \mathcal{S}$. The exclusion volume $w_{i,j}$ is defined by the geometrical relation $\underline{r}_i - \underline{r}_j \in w_{i,j} \Leftrightarrow$ overlap between needles of type i and j whose centers are located at $\underline{r}_i$ and $\underline{r}_j \in \mathbb{R}^2$ respectively. This model differs from the cases considered before in that $w_{i,j}$ is no longer a disc with radius R_{ij}. Note however that $w_{i,j}$ is still convex and $w_{i,i}$ a set of measure zero. The changes in the $w_{i,j}$ therefore do not really matter in the analysis.

An interesting question is what happens when the orientations are not discretized and θ is a continuous variable, $\theta \in [0, \pi]$. It is now natural to consider the system as a one component fluid with fugacity z. We expect that for $z \gg 1$ the system (at least in three and higher dimension) will have a long range orientational order with a continuum of extremal Gibbs states μ_θ. We are unfortunately unable to prove this with present methods.

Starting with finite n we may consider surrounding each θ_α by an interval δ, i.e. we let θ take values in $\delta_\alpha = (\theta_\alpha - \delta/2, \theta_\alpha + \delta/2)$, $\alpha \in \mathcal{S}_\alpha$. It seems likely that our analysis can be carried through for the case when $\delta \ll \operatorname{Min}_{i,j \in \mathcal{S}} |\theta_i - \theta_j|$. Other extensions are also possible but the full rotational problem awaits some new ideas.

4. We mention finally that our results can be extended to prove the positivity of the surface tension between two coexisting phases of the Widom-Rowlinson system [1].

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Note Added in Proof

We have further extended our generalizations of Pirogov-Sinai theory and can now answer affirmatively the question raised at the end of Sect. 6.2.