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EXISTENCE THEOREMS FOR CLASSICAL HETEROPHASE SYSTEMS

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A rigorous definition of a classical heterophase system is proposed,and formulations of basic theorems on existence of heterophase systems, their ergodic properties, and the possibility of gibbsian description of such systems are given.

The investigation has been performed at the Laboratory of Computing Techniques and Automation, JINR.

Теоремы существования для классических гетерофазных систем

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Предлагается строгое определение классической гетерофазной системы и приводятся формулировки основных теорем о существовании гетерофазных систем, их эргодических свойствах и возможности гиббсовского описания таких систем.

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Let us recollect physical conclusions on the nature of heterophase systems

(a) A heterophase system describes a certain "mixture" of pure thermodynamical phases.

(b) The mixture in (a) is to be understood in the sense that configurations typical of the heterophase system consist of pieces of configurations typical of the pure phases forming that system.

(c) Though local fluctuations are possible, there exist definite concentrations with which the pieces of configurations in (b) are met in the infinite volume limit.

(d) A heterophase system itself should be macroscopically observable, in the usual sense of equilibrium statistical mechanics.

In this note we propose a rigorous definition of a heterophase system and announce a number of existence theorems for such systems. We suppose reader's familiarity with basic concepts of ergodic theory /3/ and the standard frame of equilibrium statistical mechanics of classical (as opposed to quantum) infinite systems /4/.

Let T be a countable set. An S-valued random field $X=(X_t; t\in T)$ on T is a family of random variables defined on a common probability space ($(\Omega, \mathcal{F}, \mu)$, say) and taking values in S, which we assume to be a countable discrete set. If $T=Z^d$ (the d-dimensional integer lattice; $d\geq 1$), we let $\mathcal{P}(S)$ ($\mathcal{M}(S)$, $\mathcal{E}(S)$) denote the set of all Borel probability measures on S^T, which serve as distributions of all (of all translationally invariant, of all translationally ergodic) random fields on T.

Given a set $\{\phi^{(i)}: i\in I\}\subset S^T$ (I is a countable set interpreted as the set indexing possible pure phases), we say that the configuration $\phi^{(i)}$ meets a configuration $\phi\in S^T$ with concentration γ_i ($0\leq\gamma_i\leq 1$) if for any sequence of finite volumes V_n with $V_n\uparrow T$ we have

$$\lim_{n\to\infty} |V_n|^{-1}\ |\{t\in V_n : \phi(t)=\phi^{(i)}(t)\}| = \gamma_i .$$

Let $\mathcal{P}=\{P^{(i)}: i\in I\}\subset \mathcal{P}(S)$, and let $\gamma=(\gamma_i)_{i\in I}$ be a probability vector with at least two non-zero entries (in symbols, $\gamma\in\Gamma$). Let supp $P^{(i)}$ denote the support of the measure $P^{(i)}$, $i\in I$. A measure $P\in\mathcal{P}(S)$ is said to be a heterophase system composed of the set $\mathcal{P}$ of pure phases with concentrations γ, in symbols, $P\in\mathcal{H}(\mathcal{P},\gamma)$, if

$$P\Big(\bigcap_{i\in I}\ \bigcup_{\phi^{(i)}\in \operatorname{supp} P^{(i)}} R(\phi^{(i)}, \gamma_i)\Big)=1 ,$$

where $R(\phi^{(i)},\gamma_i)$ is the set of all configurations $\phi\in S^T$ described above.

<u>Theorem 1</u>. Let $\mathcal{P}=\{P^{(i)}: i\in I\}$ be the set of distributions of a jointly stationary class $\{X^{(i)}: i\in I\}$ of random fields on $T=Z^d$. Then $\mathcal{M}(S)\cap\mathcal{H}(\mathcal{P},\gamma)\neq\emptyset$ for any $\gamma\in\Gamma$. The proof uses the following construction of the heterophase random field $X=(X_t; t\in T)$:

$$X_t(\omega)=X_t^{(Z_t(\omega))}(\omega),\quad \omega\in\Omega,\ \ t\in T, \tag{1}$$

where $Z=(Z_t; t\in T)$ is an I-valued random field on T, independent of the family $\{X^{(i)}: i\in I\}$. In order to guarantee given concentrations $\gamma\in\Gamma$, it is necessary to impose the additional condition that $Z\in\mathcal{E}(I)$. Of course, this result does not say anything about property (d) which is, as is well known, related to ergodic properties of the random field X. If we strengthen requirements on the fields $X^{(i)}$, we shall get a stronger conclusion as well:

Theorem 2. Let $\mathcal{P} = \{P^{(i)} : i \in I\}$ be the set of distributions of a jointly weak mixing set $\{X^{(i)} : i \in I\}$ of random fields on $T = Z^d$. Then $\mathcal{E}(S) \cap \mathcal{H}(\mathcal{P}, \gamma) \neq \phi$ for any $\gamma \in \Gamma$. Suppose $P \in \mathfrak{M}(S) \cap \mathcal{H}(\mathcal{P}, \gamma)$ (see Theorem 1). Then Theorem 2 can be obtained also without imposing the weak mixing condition with the aid of the ergodic decomposition [3,5] $\langle f \rangle_P = \int \langle f \rangle P_\phi P(d\phi)$.

Indeed, if $P \in \mathfrak{M}(S) \cap \mathcal{H}(\mathcal{P}, \gamma)$, then

$$P\{\phi \in S^T : P_\phi \in \mathcal{E}(S) \cap \mathcal{H}(\mathcal{P}, \gamma)\} = 1 . \qquad (2)$$

Using the decomposition at infinity [5] we can guarantee even existence of random fields with trivial tails (of course, they will not longer be translationally invariant):

Theorem 3. If $\mathfrak{M}(S) \cap \mathcal{H}(\mathcal{P}, \gamma) \neq \phi$ then there exists a $P \in \mathcal{H}(\mathcal{P}, \gamma)$ having trivial tail σ-field. Hence, heterophase systems with broken symmetry but possessing short-range correlations [6] exist.

In our subsequent considerations we shall suppose that $S = \{0,1\}$. All concepts used without special comments are to be found in [6].

Theorem 4. Let $\mathcal{P} = \{P^{(i)} : i \in I\}$ be the set of distributions of a set of Markov fields $\{X^{(i)} : i \in I\}$ on $T = Z^d$. Let Z be an I-valued random field on T, independent of the family $\{X^{(i)} : i \in I\}$ such that its distribution is strictly positive on all finite cylinders in S^T. Then the random field X (cf.(1)) is Markov. More generally, if $X^{(i)}$ is $R^{(i)}$-Markov and if $\sup R^{(i)} \leq R < \infty$, then X is R-Markov. Using the well-known corresponsence between Markov field and Gibbs fields we get from this the following result. Here, $\mathcal{G}(U)$ stands for the set of all Gibbs measures to a potential U [6].

Theorem 5. Let $\mathcal{P} = \{P^{(i)} : i \in I\}$, where $P^{(i)} \in \mathcal{G}(U^{(i)})$, and $U^{(i)}$ is a nearest neighbour potential for each $i \in I$. If the remaining hypotheses of Thm.4 are satisfied, then there exists a nearest neighbour potential U such that $P = \mathrm{dist}(X)$ (cf. (1); $\mathrm{dist}(X)$ will denote the distribution of X) is in $\mathcal{G}(U)$.

Let $\mathrm{Ext}\,\mathcal{G}(U)$ denote the set of all extreme points of the convex set $\mathcal{G}(U)$. It is commonly accepted (on the base of correlation properties) that $P \in \mathrm{Ext}\,\mathcal{G}(U)$ may serve as a completely satisfactory description of "macroscopic observability". Consequently, it is of interest to have the following result:

Theorem 6. Let $\{P^{(i)} : i \in I\}$, $\{X^{(i)} : i \in I\}$, Z , and X be as in Theorems 4 and 5. Furthermore, suppose that Z is mixing and $P^{(i)} \in \mathrm{Ext}\, \mathcal{G}(U^{(i)})$ for each $i \in I$. Then there exists a nearest neighbour potential U such that $P = \mathrm{dist}(X) \in \mathrm{Ext}\, \mathcal{G}(U)$. In particular, for any $\gamma \in \Gamma$ there is a potential U such that $\mathrm{Ext}\, \mathcal{G}(U) \cap \mathcal{H}(\mathcal{P}, \gamma) \neq \emptyset$.

Theorems 1 through 6 show there exist heterophase systems which correspond to

(1) a symmetry preserving phase transition (i.e., non-uniqueness of the infinite-volume Gibbs measure for a given potential such that all these measures obey the same symmetry group),

as well as to

(b) phase transition as a spontaneous symmetry breaking (i.e., existence of Gibbs measures with a given symmetry group as well as ones having lower (broken) symmetry).

On the other hand, they are merely existence results, and an explicit calculation of the corresponding "heterophase" potentials is not possible using these theorems.

Let us consider the model of Gibbs fields on infinite trees /6,7/. Its advantage is that one can calculate a phase transition directly by giving the distributions of different pure phases. We consider again $S = \{0, 1\}$ and $T = T_3$, where T_3 is the infinite tree such that each of its sites coincides with exactly three branches. If t is a given site, we let t_1, t_2, t_3 generically denote its neighbouring sites. A Markov random field (MRF) on T_3 has its conditional probabilities uniquely determined by the vector $a = (a_0, a_1, a_2, a_3)$, where

$$a_k = P[X_t = 1 \mid |\{j : X_{t_j} = 1\}| = k], \quad 0 \leq k \leq 3 . \tag{3}$$

If U is a homogeneous nearest neighbour potential, i.e., if $U(s, t) = v_0$ for $s = t$, $U(s, t) = v_1$ if s , t are neighbours, and $U(s, t) = 0$ otherwise, then any $P \in \mathcal{G}(U)$ will possess conditional probabilities

$$a_k = [1 + \exp(\frac{v_0}{2} + kv_1)]^{-1} , \quad 0 \leq k \leq 3 .$$

As is shown in /6,7/ , conversely, knowing (3) we can reconstruct the potential U as well as find explicit expressions for finite-dimensional distributions of the corresponding random fields.

If $v_0 = 0$, $v_1 > 0$ then $|\mathcal{G}(U)| > 1$, i.e., a phase transition occurs. Let $\mathcal{P} = \{P^{(1)}, P^{(2)}\}$, where $P^{(1)}, P^{(2)} \in \mathrm{Ext}\, \mathcal{G}(U)$, let $X^{(1)}$, $X^{(2)}$ denote the corresponding random fields. We consider the random field X defined by the construction (1), where $Z=(Z_t; t\in T_3)$ is a family of i.i.d. random variables such that $P[Z_t=0]=\gamma_1=1-P[Z_t=1]$, $t\in T_3$. Then $P=\mathrm{dist}(X)\in \mathcal{H}(\mathcal{P},\gamma)$. It is easy to see that X is again a MRF on T_3 and it is possible (although rather cumbersome) to calculate its parameters $\tilde{a}$ (see (3)) as functions of the "old" parameters a and of $\gamma=(\gamma_1, 1-\gamma_1)$. Consequently, we can calculate the "heterophase" potential as well: $\tilde{U}=\tilde{U}(v_1,\gamma_1)$. We have the following surprising result:

Theorem 7. There exists a constant $v^*>0$ such that for any $0<v_1<v^*$ there is a $\gamma=(\gamma_1, 1-\gamma_1)\in\Gamma$ for which $|\mathcal{G}(\tilde{U})|=1$, where $\tilde{U}=\tilde{U}(v_1,\gamma_1)$. In orher words, the heterophase potential does not admit a phase transition.

The complete proofs of all these results together with an analysis of more realistic model systems will appear elsewhere.

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