

A Variational Principle for General Polymer Systems

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Es wird ein neues Modell für die klassische statistische Mechanik von wechselwirkenden ausgedehnten Teilchen (Polymeren) eingeführt. Für Systeme von Polymeren wird die Konstruktion des Konfigurationsraumes angegeben. Es folgt der Nachweis für die Existenz des thermodynamischen Grenzwertes des lokalen Drucks. Für diesen Grenzwert, den Druck des Systems, wird ein Variationsprinzip bewiesen. Abschließend wird gezeigt, daß bei gegebener Wechselwirkung die Klasse der Gleichgewichtszustände, die durch das Variationsprinzip beschrieben wird, mit der Klasse der verschiebungsinvarianten Gibbsschen Zustände zusammenfällt.

Введётся новая модель для классической статистической механики взаимодействующих пространственных частиц (полимеров). Для систем полимеров описывается конструкция конфигурационного пространства. Потом следует доказательство существования термодинамического предела локального давления. Для этого предела, так называемого давления системы, доказывается вариационный принцип. Заключительно доказывается, что при данном взаимодействии класс равновесных состояний, описываемый этим вариационным принципом, совпадает с классом трансляционно-инвариантных гиббсовских состояний.

A new model for classical statistical mechanics of interacting extended particles (polymers) is introduced. First, the construction of the configuration space for polymer systems is given. Then the existence of the thermodynamic limit of the local pressure is derived. For this limit which is called the pressure of the system a variational principle is proved. Finally, for given interaction, the class of equilibrium states determined by this variational principle is proved to coincide with the class of translation invariant Gibbs states.

1. Introduction

Exactly soluble models are of great importance in the understanding of statistical mechanics of phase transitions. Besides the classical models, general hard core or polymer models are of interest, too [1, 5–9]. In these models the particles of the system can cover more than one lattice point of the underlying lattice without penetrating each other. The most interesting examples are hard-rod models. They have been widely used to explain the existence of liquid crystals. Thus the theory of monomer-dimer systems is elaborated extensively [1, 7–9]. In [8] the reader can find more details about the relation of these models to chemistry and physics.

Most results are known for models without interaction between the particles; but a successful approach to the practical models requires models with interaction. In [8] the absence of a phase transition is proved for translationally invariant systems of non-interacting monomers and dimers on the lattice Z^d . In [5] GRUBER and KUNZ incorporated into their model particles that are more complicated with respect to their geometry. They showed the absence of a phase transition for non-interacting polymers and thus generalized the results by HEILMANN and LIEB in [8]. In [9] HEILMANN and LIEB succeeded in a rigorous proof of the existence of a phase transition for monomer-dimer systems with two-body interactions between the dimers in two dimensions. A similar result can be found in [1] for three dimensions.

In our paper we describe a very general model for systems of polymers that can interact via many-body interactions. The underlying lattice is \mathbf{Z}^d for $d \geq 1$, and the polymers have the shape of finite subsets of the lattice. It is possible to have different polymers of the same shape, but only finitely many shapes of polymers are allowed in the system. We found this model in specifying the general method for the construction of configuration spaces of classical lattice systems of RUELLE in [13].

The proof of the variational principle for the pressure of the system [4, 10] was a milestone in the development of classical statistical mechanics. This result influenced not only statistical mechanics, but also ergodic theory. It was one basis for the further development of entropy theory, especially for the generalization of the variational principle for the entropy, which asserts that the topological entropy of a continuous transformation of a compact space is the supremum of the measure-theoretic entropies of regular invariant probability measures. As one generalization of entropy, RUELLE developed the concept of the pressure of a continuous transformation of a compact space in [12]. For further results in ergodic theory see [2, 3, 13] and references therein. Some definitions and theorems that are used in our paper are summarized in the Appendix.

In the second part we introduce our model. The third part is devoted to the proof of the existence of the pressure $P(U)$ for systems of interacting polymers with interaction U and to the proof of a variational principle

$$P(U) = \sup_{\mu \in \mathcal{J}} |\mathcal{S}_0|^{-1} (h(\mu) - \mu(U)).$$

Herein $h(\mu)$ denotes the entropy of the invariant state μ , $\mu(U)$ the specific energy of the system, $|\mathcal{S}_0|^{-1}$ the number of different shapes that polymers are allowed to have. Knowing that this variational principle is true for a particle system, the problem of phase transition reduces to the question: Does there exist more than one state μ being an equilibrium state, in the sense that it fulfils the equation

$$P(U) = |\mathcal{S}_0|^{-1} (h(\mu) - \mu(U))?$$

A uniqueness theorem, i.e. a theorem about the absence of a phase transition for some systems of interacting particles, was published in [15]. In the fourth part it is shown that the class of equilibrium states coincides with the class of translation invariant Gibbs states for the given polymer system with interaction U .

2. The model

We start with the construction of the configuration space of the polymer system. Let \mathbf{Z}^d be the set of all d -tuples of integers $s = (s_1, \dots, s_d)$, $\mathfrak{P}_f(\mathbf{Z}^d)$ the set of all non-empty finite subsets of \mathbf{Z}^d . We choose a set $\mathcal{S} \subset \mathfrak{P}_f(\mathbf{Z}^d)$ of possible polymer shapes such that for each $s \in \mathbf{Z}^d$ the set $\mathcal{L}_s = \{G \in \mathcal{S} \mid s \in G\}$ is non-empty and finite. Furthermore we choose for each $G \in \mathcal{S}$ a finite set Ω_G of possible species of polymers of the shape G and assume that there is an element $O \in \Omega_G$ for each $G \in \mathcal{S}$. Let $\bar{\Omega}_s = \prod \{\Omega_G \mid G \in \mathcal{L}_s\}$ be the set defined by

$$\bar{\Omega}_s = \bigcup_{G \in \mathcal{L}_s} \bigcup_{\omega_G \in \Omega_G} \{(0, \dots, 0, \omega_G, 0, \dots, 0)\}.$$

The configuration space Ω for the polymer model is defined by

$$\Omega = \left\{ \omega \in \prod_{G \in \mathcal{S}} \Omega_G \mid \omega|_{\mathcal{L}_s} \in \bar{\Omega}_s, \text{ for all } s \in \mathbf{Z}^d \right\}.$$

The space Ω consists of configurations ω having the property that for any point $s \in \mathbf{Z}^d$ there exists at most one $G \in \mathcal{L}_s$ with $\omega|_G \neq 0$.

So it will be convenient to interpret the configurations as arrangements of non-overlapping polymers on the lattice. The construction of the configuration space includes also the classical case of a lattice gas. To see this, choose the parameters as $\mathcal{S} = \{\{s\} \mid s \in \mathbf{Z}^d\}$ and $\Omega_{\{s\}} = \{0, 1\}$. A more abstract definition of configuration spaces with restrictions is given in [13]. Our model arises from this approach.

In the following, invariance under the group $(\Theta_s)_{s \in \mathbf{Z}^d}$ of translations acting on the lattice by

$$\Theta_s t = t - s \quad (t \in \mathbf{Z}^d)$$

is assumed. The translate of sets $W \in \mathfrak{P}_r(\mathbf{Z}^d)$ or $\mathcal{W} \subset \mathfrak{P}_r(\mathbf{Z}^d)$ is denoted by $\Theta_s W$ or $\Theta_s \mathcal{W}$, respectively. The set \mathcal{S} is supposed to be uniquely generated by (Θ_s) from a finite set \mathcal{S}_0 chosen in such a way that the origin of \mathbf{Z}^d is in the lexicographic order the smallest element in each $G \in \mathcal{S}_0$. Furthermore we assume that $\Omega_G = \Omega_K$ if $G = \Theta_s K$ for some $s \in \mathbf{Z}^d$.

The configuration space Ω is to be equipped with a metric. For this let $|s| = \max \{|s_1|, \dots, |s_d|\}$ for $s = (s_1, \dots, s_d) \in \mathbf{Z}^d$ and $d(G) = \min \{|s| \mid s \in G\}$ for $G \in \mathcal{S}$. Then for each $\vartheta \in (0, 1)$ a metric ρ_ϑ on Ω is defined by

$$\rho_\vartheta(\omega, \eta) = \exp \left(\left(\inf_{G \in \mathcal{S}} \{d(G) \mid \omega|_G \neq \eta|_G\} \right) \log \vartheta \right). \quad (1)$$

This metric is compatible with the topology induced on $\Omega \subset \prod \{\Omega_G \mid G \in \mathcal{S}\}$ by the product topology on $\prod \Omega_G$. On finite sets Ω_G the discrete topology is assumed. So Ω is seen to be compact and metrizable. On Ω the expansive group (see Appendix) $(\tau_s)_{s \in \mathbf{Z}^d}$ of homeomorphisms τ_s is defined by

$$\tau_s \omega|_G = \omega|_{\Theta_{-s} G} \quad (\omega \in \Omega, s \in \mathbf{Z}^d, G \in \mathcal{S}).$$

The set of all Borel probability measures on Ω , the so-called *states*, is denoted by \mathcal{M} , while all translation invariant elements of \mathcal{M} form the set \mathcal{I} .

For the proofs of the theorems we use some results of ergodic theory. They are shortly summarized in the Appendix.

3. Thermodynamic limit and variational principle

In this part we introduce interactions for systems of polymers and prove first the existence of the thermodynamic limit of the local pressure. For this limit which is called *pressure of the system* the variational principle is verified. The methods of the proofs are very close to those used in [13: Chap. 3].

Given $a \in \mathbf{Z}^{+d} = \{s \in \mathbf{Z}^d \mid s_i \geq 0 \text{ for all } i\}$, we write

$$V(a) = \{s \in \mathbf{Z}^d \mid |s_i| \leq a_i \text{ for all } i\}, \quad \mathcal{V}(a) = \{G \in \mathcal{S} \mid G \cap V(a) \neq \emptyset\}.$$

The cardinality of sets $V \in \mathfrak{P}_r(\mathbf{Z}^d)$ or $\mathcal{V} \subset \mathfrak{P}_r(\mathbf{Z}^d)$ is denoted by $|V|$ or $|\mathcal{V}|$, respectively, while $[\mathcal{V}]$ denotes

$$[\mathcal{V}] = \cup \{\Theta_s \mathcal{V} \mid s \in \mathbf{Z}^d\}.$$

For $G \in \mathcal{S}_0$ it is possible to introduce an order relation in the set $\{[G]\}$ in the following way: Take on \mathbf{Z}^d the lexicographic order " \leq " and set $G_1 \leq G_2$ if $G_1 = \Theta_s G_2$

and $G_2 = \Theta_t G$ with $s \leq t$. The set of non-empty finite subsets of \mathcal{S} is denoted by $\mathfrak{P}_f(\mathcal{S})$.

An *interaction* is a map $U: \mathfrak{P}_f(\mathcal{S}) \times \Omega \rightarrow \mathbf{R}$ such that for fixed $\mathcal{V} \in \mathfrak{P}_f(\mathcal{S})$ the value $U(\mathcal{V}, \omega)$ depends only on $\omega|_{\mathcal{V}}$. An interaction U is *translation invariant* if

$$U(\mathcal{V}, \omega) = U(\Theta_s \mathcal{V}, \tau_s \omega) \quad (\mathcal{V} \in \mathfrak{P}_f(\mathcal{S}), \omega \in \Omega, s \in \mathbf{Z}^d).$$

The set $(\mathfrak{R}, \|\cdot\|)$ of translation invariant interactions U with

$$\|U\| = \sum_{G \in \mathcal{S}_0} \sum_{\substack{\mathcal{V} \in \mathfrak{P}_f(\mathcal{S}) \\ \mathcal{S} \in \mathcal{V}}} |\mathcal{V} \cap \{G\}|^{-1} \sup_{\omega \in \Omega} |U(\mathcal{V}, \omega)| < \infty$$

is a Banach space. The same is true for the set $\mathfrak{S} \subset \mathfrak{R}$ with the norm

$$\| \|U\| \| = \sum_{G \in \mathcal{S}_0} \sum_{\substack{\mathcal{V} \in \mathfrak{P}_f(\mathcal{S}) \\ \mathcal{S} \in \mathcal{V}}} \sup_{\omega \in \Omega} |U(\mathcal{V}, \omega)|.$$

A translation invariant interaction U is of *finite range*, $U \in \mathfrak{R}_0$, if there exists a set $\mathcal{D} \in \mathfrak{P}_f(\mathcal{S})$ with $\mathcal{D} \cap \mathcal{S}_0 \neq \emptyset$ such that $U(\mathcal{V}, \cdot) \equiv 0$ implies the existence of an $s \in \mathbf{Z}^d$ with $\Theta_s \mathcal{V} \subset \mathcal{D}$.

For $\mathcal{V} \in \mathfrak{P}_f(\mathcal{S})$ the *projection* of Ω into the set $\prod \{\Omega_G \mid G \in \mathcal{V}\}$ is denoted by $X_{\mathcal{V}} \Omega$.

For $\mathcal{V} \subset \mathcal{S}$ finite and $U \in \mathfrak{R}$ we define the *partition function* $Z_{\mathcal{V}}(U)$ by

$$Z_{\mathcal{V}}(U) = \sum_{\omega \in X_{\mathcal{V}} \Omega} \exp \left(- \sum_{\mathcal{Y} \subset \mathcal{V}} U(\mathcal{Y}, \omega^*) \right),$$

where ω^* is an arbitrary configuration with $\omega^*|_{\mathcal{V}} = \omega$. By the definition of an interaction the partition function does not depend on the special choice of ω^* .

The *local pressure* is defined by

$$P_{\mathcal{V}}(U) = |\mathcal{V}|^{-1} \log Z_{\mathcal{V}}(U) \quad (\mathcal{V} \in \mathfrak{P}_f(\mathcal{S}), U \in \mathfrak{R}).$$

Our aim is to prove the existence of the thermodynamic limit of the local pressure, i.e. the existence of $\lim_{a \rightarrow \infty} P_{\mathcal{V}(a)}(U)$ as $a \rightarrow \infty$. For proving this, to each $U \in \mathfrak{R}$ we adjoin a continuous function $A_U: \Omega \rightarrow \mathbf{R}$ by

$$A_U(\omega) = - \sum_{G \in \mathcal{S}_0} \sum_{\substack{\mathcal{V} \in \mathfrak{P}_f(\mathcal{S}) \\ \mathcal{V} \in G}}^* |\mathcal{V} \cap \mathcal{S}_0|^{-1} U(\mathcal{V}, \omega).$$

Here the second summation means that we sum up only those sets $\mathcal{V} \in \mathfrak{P}_f(\mathcal{S})$ for which G is the G -greatest element in \mathcal{V} with respect to the order " \leq " in $\{G\}$. It is not hard to see that $U \rightarrow A_U$ is a linear and continuous map from \mathfrak{R} into the set $\mathcal{E}(\Omega)$ of all continuous real functions on Ω equipped with the sup-norm. But this map is furthermore onto. We verify this in two steps:

1. For $\mathcal{V} \in \mathfrak{P}_f(\mathcal{S})$ let $\mathcal{E}_{\mathcal{V}}$ be the algebra of real functions on Ω depending only on $\omega|_{\mathcal{V}}$. It is then clear that $\{A_U \mid U \in \mathfrak{R}_0\}$ is a subset of $\cup \{\mathcal{E}_{\mathcal{V}} \mid \mathcal{V} \in \mathfrak{P}_f(\mathcal{S})\}$, which is dense in $\mathcal{E}(\Omega)$. For the demonstration of the inverse inclusion take an arbitrary $\mathcal{V} \in \mathfrak{P}_f(\mathcal{S})$, an $A \in \mathcal{E}_{\mathcal{V}}$ and an $a \in \mathbf{Z}^{+d}$ such that $\mathcal{V}(a) \supset \mathcal{V}$. Adjoin to A the interaction $U \in \mathfrak{R}_0$ by

$$U(\mathcal{V}(a), \omega) = -A(\tau_a \omega) \quad (\omega \in \Omega),$$

$$U(\mathcal{V}, \omega) = -A(\tau_{a-s} \omega) \quad \text{if } \mathcal{V} = \Theta_s \mathcal{V}(a) \quad (\omega \in \Omega),$$

$$U(\mathcal{V}, \omega) = 0 \quad \text{if } \mathcal{V} \notin [\mathcal{V}(a)] \quad (\omega \in \Omega).$$

A short calculation shows that $A_U = A$. Moreover, the equality $\|U\| = |\mathcal{S}_0| \|A\|$ holds.

2. Let $A \in \mathcal{E}(\Omega)$. Because of the continuity of A one can choose an increasing sequence $(V_n) \subset \mathfrak{P}_f(\mathcal{S})$ such that

$$\sup \{ |A(\omega) - A(\eta)| \mid \omega, \eta \in \Omega \text{ with } \omega|_{V_n} = \eta|_{V_n} \} < \frac{1}{2^n}.$$

For $\omega \in \Omega$ and $n \in \mathbb{N}$ we set

$$B_n(\omega) = A(\omega|_{V_n, 0}) \quad \text{and} \quad A_1 = B_1, \quad A_n = B_n - B_{n-1},$$

where $\omega|_{V_n, 0}$ is the configuration η with $\eta|_{V_n} = \omega|_{V_n}$ and $\eta|_{\mathcal{S} \setminus V_n} \equiv 0$. To the functions $A_n \in \mathcal{E}_{V_n}$ interactions $U_n \in \mathfrak{R}_0$ are adjoined as described in Step 1, to the function A the interaction $U = \sum U_n$. This procedure yields

$$\begin{aligned} A_U(\omega) &= - \sum_{G \in \mathcal{S}_0} \sum_{\substack{v \in \mathfrak{P}_f(\mathcal{S}) \\ G \in V}}^* |V_n \cap \mathcal{S}_0|^{-1} \left(\sum_n U_n(V, \omega) \right) \\ &= \sum_n A_n(\omega) = A(\omega) \quad (\omega \in \Omega). \end{aligned}$$

The next inequality shows that U is indeed an element of \mathfrak{R} :

$$\|U\| = \left\| \sum_n U_n \right\| \leq \sum_n \|U_n\| = \sum_n |\mathcal{S}_0| \|A_n\| < \infty \quad \blacksquare$$

The *partition functions* in the finite volumes $V \in \mathfrak{P}_f(\mathbb{Z}^d)$ for continuous functions A and expansiveness constants $\varepsilon > 0$ are defined (see Appendix) by

$$Z_V(A, \varepsilon) = \sup \left\{ \sum_{\omega \in A} \exp \left(\sum_{s \in V} A(\tau_s \omega) \right) \mid A \text{ is } (V, \varepsilon)\text{-separated} \right\}.$$

We mentioned above that the group (τ_s) is expansive. This is true especially for the expansiveness constant $\varepsilon = \vartheta$ (see (1)). It is not hard to show that for $a \in \mathbb{Z}^{+d}$ the $(V(a), \vartheta)$ -separated subsets $A \subset \Omega$ have the property

$$\omega, \eta \in A \quad \text{and} \quad \omega \neq \eta \Rightarrow \omega|_{V(a)} \neq \eta|_{V(a)}.$$

So we can write the partition function in $V(a)$ for A and $\varepsilon = \vartheta$ in the form

$$Z_{V(a)}(A) = \sum_{\omega \in X_{V(a), \vartheta}} \exp \left(\sum_{s \in V(a)} A(\tau_s \omega^*) \right),$$

where the configurations ω^* with $\omega^*|_{V(a)} = \omega$ form that $(V(a), \vartheta)$ -separated set A that gives the supremum in $Z_{V(a)}(A, \vartheta)$. It is known (see Appendix) that the thermodynamic limit

$$\lim_{a \rightarrow \infty} |V(a)|^{-1} \log Z_{V(a)}(A) = P(A)$$

exists for all $A \in \mathcal{E}(\Omega)$, and because of $|V(a)|/|V(a)| \rightarrow |\mathcal{S}_0|$ as $a \rightarrow \infty$ there exists also the limit

$$\lim_{a \rightarrow \infty} |V(a)|^{-1} \log Z_{V(a)}(A) = |\mathcal{S}_0|^{-1} P(A).$$

Theorem 1: *For each interaction $U \in \mathfrak{R}$ the thermodynamic limit*

$$\lim_{a \rightarrow \infty} |V(a)|^{-1} \log Z_{V(a)}(U) = \lim_{a \rightarrow \infty} P_{V(a)}(U) = |\mathcal{S}_0|^{-1} P(A_U)$$

exists and is called the pressure $P(U)$ of U .

Proof: 1. Let U be of finite range and let \mathcal{D} be the set determining the range of U . If $a \in \mathbf{Z}^d$ is sufficiently large and $N(\mathcal{V}(a)) = |\{s \in V(a) \mid \Theta_s \mathcal{D} \not\subset \mathcal{V}(a)\}|$, then for all $\omega \in \Omega$

$$\begin{aligned} & \left| \sum_{\mathcal{Y} \subset \mathcal{V}(a)} U(\mathcal{Y}, \omega) + \sum_{s \in V(a)} A_{\sigma}(\tau_s \omega) \right| \\ &= \left| \sum_{G \in \mathcal{S}_0} \sum_{\substack{\mathcal{Y} \in \mathfrak{P}_1(\mathcal{S}) \\ G \in \mathcal{Y}}}^* |\mathcal{Y} \cap \mathcal{S}_0|^{-1} \left(\sum_{\substack{s \in \mathbf{Z}^d \\ \Theta_s \mathcal{Y} \supset \mathcal{V}(a)}} U(\mathcal{Y}, \tau_s \omega) - \sum_{s \in V(a)} U(\mathcal{Y}, \tau_s \omega) \right) \right| \\ &\leq N(\mathcal{V}(a)) \sum_{G \in \mathcal{S}_0} \sum_{\substack{\mathcal{Y} \in \mathfrak{P}_1(\mathcal{S}) \\ \mathcal{S} \in \mathcal{Y}}}^* |\mathcal{Y} \cap \mathcal{S}_0|^{-1} \sup_{\omega \in \Omega} |U(\mathcal{Y}, \omega)| \leq N(\mathcal{V}(a)) \|U\|. \end{aligned} \tag{2}$$

Because of $N(\mathcal{V}(a))/|\mathcal{V}(a)| \rightarrow 0$ as $a \rightarrow \infty$, one can calculate

$$\begin{aligned} & \lim_{a \rightarrow \infty} |\mathcal{V}(a)|^{-1} |\log Z_{\mathcal{V}(a)}(U) - \log Z_{\mathcal{V}(a)}(A_U)| \\ &= \lim_{a \rightarrow \infty} |\mathcal{V}(a)|^{-1} \left| \log \frac{\sum_{\omega \in \mathcal{X}_{\mathcal{V}(a)}^{\Omega}} \exp\left(-\sum_{\mathcal{Y} \subset \mathcal{V}(a)} U(\mathcal{Y}, \omega^*)\right)}{\sum_{\omega \in \mathcal{X}_{\mathcal{V}(a)}^{\Omega}} \exp\left(-\sum_{s \in V(a)} A(\tau_s \omega^*)\right)} \right| \\ &\leq \lim_{a \rightarrow \infty} |\mathcal{V}(a)|^{-1} N(\mathcal{V}(a)) \|U\| = 0. \end{aligned}$$

This proves the theorem for $U \in \mathfrak{R}_0$.

2. For an arbitrary $U \in \mathfrak{R}$ we take into account that for $U' \in \mathfrak{R}$, $t \in \mathbf{R}$ and $a \in \mathbf{Z}^d$

$$\left| \frac{d}{dt} P_{\mathcal{V}(a)}(U + tU') \right| \leq \|U\| |V(a + c)|/|\mathcal{V}(a)|$$

holds with $c \in \mathbf{Z}^d$ defined by $c_i = \max \{|s_i - t_i| \mid s \in G', t \in G'' \text{ for some } G', G'' \in \mathcal{S}_0\}$, $i = 1, \dots, d$. This yields

$$\begin{aligned} |P_{\mathcal{V}(a)}(U) - P_{\mathcal{V}(a)}(U')| &\leq \sup_{-1 \leq t \leq 1} \left| \frac{d}{dt} P_{\mathcal{V}(a)}(U + t(U' - U)) \right| \\ &\leq \|U - U'\| |V(a + c)|/|\mathcal{V}(a)|. \end{aligned}$$

Because of $|V(a + c)|/|\mathcal{V}(a)| \rightarrow |\mathcal{S}_0|^{-1}$ as $a \rightarrow \infty$ and the possibility to approximate U by elements $U' \in \mathfrak{R}_0$, the last estimate ensures the existence of the thermodynamic limit of the local pressure of U . From the continuity of the maps $U \rightarrow A_U$ and $A \rightarrow P(A)$ we deduce that this limit is equal to $|\mathcal{S}_0|^{-1} P(A_U)$ ■

Theorem 2: For $\mu \in \mathcal{J}$ and $U \in \mathfrak{R}$ the finite thermodynamic limit

$$\mu(U) = \lim_{a \rightarrow \infty} |\mathcal{V}(a)|^{-1} \int \left(\sum_{\mathcal{Y} \subset \mathcal{V}(a)} U(\mathcal{Y}, \omega) \right) d\mu(\omega)$$

exists. Furthermore $\mu(U) = -\int A_U(\omega) d\mu(\omega)$.

Proof: For $U \in \mathfrak{R}_0$ the theorem follows from a multidimensional version of Birkhoff's ergodic theorem (see [14]) and inequality (2). An interaction $U \in \mathfrak{R}$ can again be approximated by interactions of \mathfrak{R}_0 ■

In the situation of polymer systems the *entropy* $h(\mu)$ of a state $\mu \in \mathcal{J}$ (see Appendix) is calculated as

$$h(\mu) = -\lim_{a \rightarrow \infty} |V(a)|^{-1} \sum_{\omega \in X_{V(a)}\Omega} (X_{V(a)}\mu)(\omega) \log (X_{V(a)}\mu)(\omega).$$

Let \mathcal{E}^* denote the weak dual of $\mathcal{E}(\Omega)$. For $A \in \mathcal{E}(\Omega)$ we set

$$\mathcal{J}_A = \{\mu \in \mathcal{E}^* \mid P(A + B) \geq P(A) + \mu(B) \text{ for all } B \in \mathcal{E}(\Omega)\}.$$

The elements of \mathcal{J}_A are called *equilibrium states for A*, those of \mathcal{J}_{A_U} for an interaction U , *equilibrium states for U*. Now we can formulate our main result.

Variational principle: For each interaction $U \in \mathfrak{R}$,

$$P(U) = \sup_{\mu \in \mathcal{J}} \{|\mathcal{S}_0|^{-1} (h(\mu) - \mu(U))\}$$

and

$$\mathcal{J}_{A_U} = \{\mu \in \mathcal{J} \mid P(U) = |\mathcal{S}_0|^{-1} (h(\mu) - \mu(U))\}.$$

The set \mathcal{J}_{A_U} is non-empty, convex and compact.

This result follows from Theorems 1 and 2 and the next Lemma, which is due to RUELLE [13] together with the variational principle quoted in the Appendix.

Lemma: For each $A \in \mathcal{E}(\Omega)$ the following assertions are true.

- (i) $\mathcal{J}_A = \{\mu \in \mathcal{J} \mid P(A) = h(\mu) + \mu(A)\}$.
- (ii) \mathcal{J}_A is non-empty, convex and compact.
- (iii) Let \mathfrak{X} be a separable Banach space, $\varphi: \mathfrak{X} \rightarrow \mathcal{E}(\Omega)$ a continuous linear map with dense domain, and for $\Phi \in \mathfrak{X}$ define

$$\mathcal{J}_{\Phi'} = \{F \in \mathfrak{X}^* \mid P \circ \varphi(\Phi + \Psi) \geq P \circ \varphi(\Phi) + F(\Psi) \text{ for all } \Psi \in \mathfrak{X}\}.$$

Then $\mathcal{J}_{\Phi'} = \{\sigma \circ \varphi \mid \sigma \in \mathcal{J}_{\varphi\Phi}\}$.

In our special case of polymer systems one has to choose $\mathfrak{X} = \mathfrak{R}$ and $\varphi: U \rightarrow A_U$ and to mention that $\cup \{\mathcal{E}_V \mid V \in \mathfrak{P}_f(\mathcal{S})\}$ is dense in $\mathcal{E}(\Omega)$.

4. Gibbs states

In the set \mathcal{M} of all states the class of Gibbs states for a given interaction is of great interest in statistical mechanics [11]. It is our aim to show that the equilibrium states are τ_a -invariant Gibbs states and vice versa.

A state is called *Gibbs state for the interaction U* if for each finite set $V \subset \mathcal{S}$ the conditional probability that on V there is the configuration $\omega_V \in X_V\Omega$, knowing that on the set $\mathcal{S} \setminus V$ there is the configuration $\eta|_{\mathcal{S} \setminus V}$ for some $\eta \in \Omega$, is equal to

$$q_{V,\eta}^U(\omega_V) = Z_{V,\eta}^{-1}(U) \exp \left(- \sum_{\substack{Y \cap V \neq \emptyset \\ Y \in \mathfrak{P}_f(\mathcal{S})}} U(Y, \omega_V \eta|_{\mathcal{S} \setminus V}) \right)$$

with

$$Z_{V,\eta}(U) = \sum_{\substack{\omega_V \in X_V\Omega \\ \omega_V \eta|_{\mathcal{S} \setminus V} \in \Omega}} \exp \left(- \sum_{\substack{Y \cap V \neq \emptyset \\ Y \in \mathfrak{P}_f(\mathcal{S})}} U(Y, \omega_V \eta|_{\mathcal{S} \setminus V}) \right).$$

It is a known fact that the set K_U of all Gibbs states for $U \in \mathcal{E}$ is non-empty, convex and compact (see [13]).

Theorem 3: For each invariant polymer configuration space Ω on \mathbb{Z}^d the class of τ_s -invariant Gibbs states for an interaction $U \in \mathcal{G}$ coincides with the set of equilibrium states of U .

The following observation is an essential step towards the proof:

Given the configuration space Ω , one can find a $\bar{c} \in \mathbb{Z}^{+d}$ such that for all $a \in \mathbb{Z}^{+d}$ and all $\omega, \eta \in \Omega$ there exists a $\xi \in \Omega$ with the property $\omega|_{\mathcal{V}(a)} = \xi|_{\mathcal{V}(a)}$ and $\eta|_{\mathcal{S} \setminus \mathcal{V}(a+\bar{c})} = \xi|_{\mathcal{S} \setminus \mathcal{V}(a+\bar{c})}$.

Let $V = \{s \in \mathbb{Z}^d \mid s \in G \text{ for some } G \in \mathcal{G}_0\}$ and for $i = 1, \dots, d$ set $\bar{c}_i = \max \{|s_i - t_i| \mid s, t \in V\}$. The d -tuple $\bar{c} = (\bar{c}_1, \dots, \bar{c}_d)$ has the desired property. To see this take any $a \in \mathbb{Z}^{+d}$, $\omega, \eta \in \Omega$ and verify with the help of the definition of Ω that

$$\xi \in \prod_{G \in \mathcal{G}} \Omega_G \text{ with } \xi|_{|G|} = \begin{cases} \omega|_{|G|} & \text{for } G \in \mathcal{V}(a), \\ \eta|_{|G|} & \text{for } G \in \mathcal{S} \setminus \mathcal{V}(a + \bar{c}), \\ 0 & \text{otherwise} \end{cases}$$

is indeed a configuration. Now one can carry out the proof of Theorem 3 analogously to the proof of a similar theorem of RUELLE for systems with a configuration space that is a subset of $\Omega_0 \mathbb{Z}^d$ for a finite set Ω_0 (see [13: Theorem 4.2]) ■

Appendix

We summarize here some definitions and theorems of ergodic theory which are the basis for the proofs of the Theorems 1 and 2. More details can be found in [2, 3, 12, 13].

Let Ω be a compact space with metric ϱ and $(\tau_s)_{s \in \mathbb{Z}^d}$ a group of homeomorphisms on Ω isomorphic to \mathbb{Z}^d .

1. *Expansiveness:* The group (τ_s) is called *expansive* if for an $\varepsilon > 0$ and for all $\omega, \eta \in \Omega$ the implication

$$\varrho(\tau_s \omega, \tau_s \eta) \leq \varepsilon \text{ for all } s \in \mathbb{Z}^d \Rightarrow \omega = \eta$$

is true. The number ε is called *expansiveness constant*.

2. *Entropy:* For τ_s -invariant Borel probability measures μ on Ω and finite Borel partitions $\mathfrak{A} = \{\mathfrak{A}_i\}$ of Ω we set

$$H(\mu, \mathfrak{A}) = - \sum_i \mu(\mathfrak{A}_i) \log \mu(\mathfrak{A}_i), \quad \mathfrak{A}^V = \bigvee_{s \in V} \tau_s \mathfrak{A} \quad (V \in \mathfrak{F}_r(\mathbb{Z}^d)).$$

Then $h_r(\mu, \mathfrak{A}) = \lim_{a \rightarrow \infty} |V(a)|^{-1} H(\mu, \mathfrak{A}^{V(a)})$ exists. The number $h(\mu) = \sup_{\mathfrak{A}} h_r(\mu, \mathfrak{A})$ is called the *entropy* of the measure μ .

We write $\text{diam } \mathfrak{A} = \max \text{diam } \mathfrak{A}_i$, where $\text{diam } \mathfrak{A}_i$ is the diameter of \mathfrak{A}_i with respect to the metric ϱ .

3. *Proposition:* If the group (τ_s) is expansive with expansiveness constant ε , then

$$\text{diam } \mathfrak{A} \leq \varepsilon \Rightarrow h(\mu) = h_r(\mu, \mathfrak{A}).$$

4. *Partition function:* Let V be a non-empty finite subset of \mathbb{Z}^d and $\varepsilon > 0$. A finite set $A \subset \Omega$ is called (V, ε) -separated if for some $s \in V$

$$\omega, \eta \in \Omega \text{ and } \omega \neq \eta \Rightarrow \varrho(\tau_s \omega, \tau_s \eta) > \varepsilon.$$

For $A \in \mathcal{C}(\Omega)$, $V \in \mathfrak{F}_r(\mathbb{Z}^d)$ and $\varepsilon > 0$ the *partition function* $Z_V(A, \varepsilon)$ is defined by

$$Z_V(A, \varepsilon) = \sup \left\{ \sum_{\omega \in A} \exp \left(\sum_{s \in V} A(\tau_s \omega) \right) \mid A \text{ is } (V, \varepsilon)\text{-separated} \right\}.$$

5. *Pressure*: If the group (τ_s) is expansive with expansiveness constant ε and $A \in \mathcal{E}(\Omega)$, then the limit

$$P(A) = \lim_{a \rightarrow \infty} |V(a)|^{-1} \log Z_{V(a)}(A, \varepsilon)$$

exists independently of ε . The value $P(A)$ is called the *pressure of the function A*. Either $P(A) = +\infty$ for all $A \in \mathcal{E}(\Omega)$, or $P(A) < +\infty$ for all $A \in \mathcal{E}(\Omega)$. In the latter case the map $A \rightarrow P(A)$ is convex, increasing and continuous.

6. *Variational principle*: If \mathcal{J} denotes the set of all τ_s -invariant Borel probability measures on Ω and $A \in \mathcal{E}(\Omega)$, then

$$P(A) = \sup \{h(\mu) + \mu(A) \mid \mu \in \mathcal{J}\}.$$

In the case of finite pressure and expansive group (τ_s) the set

$$\mathcal{J}_A = \{\mu \in \mathcal{J} \mid P(A) = h(\mu) + \mu(A)\}$$

is non-empty, convex and compact and coincides with the set

$$\mathcal{J}_A' = \{\mu \in \mathcal{J} \mid P(A + B) \geq P(A) + \mu(B) \text{ for all } B \in \mathcal{E}(\Omega)\}.$$

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Manuskripteingang: 03. 09. 1985

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