The characterization of ground states

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Abstract

We consider limits of equilibrium distributions as temperature approaches zero, for systems of infinitely many particles, and the characterization of the support of such limiting distributions. Such results are known for particles with positions on a fixed lattice; we extend these results to systems of particles on $\mathbb{R}^n$, with restrictions on the interaction.

1 Introduction

We were looking for an explanation of the "solidity" of equilibrium states at low temperature and/or high pressure. We are very far from that goal. Below we will state some conjectures, and present proofs of some special cases.

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We will be concerned with classical Gibbs states μ_β, which are grand canonical probability distributions on a phase space Ω of infinitely many point particles with positions in n-dimensional Euclidean space $\mathbb{R}^n$, interacting through a two-body potential. In principle the interaction may or may not have a hard core. We are interested in the ground states μ_∞, which can be defined as the weak accumulation points of the family μ_β, when the inverse temperature $\beta \to \infty$. The chemical potential λ will be held fixed (and sometimes will be omitted in the notation). More precisely we would like to characterize the "ground state configurations", which constitute the union of the supports of all such $\mu_\infty = \mu_\infty(\lambda)$. And we would like to determine some simple qualitative geometric properties of these configurations. (We take advantage of the fact that in many cases of interest the Gibbs state factors into distributions on the momenta and on the position variables, and that the distribution on the momenta is easily understood. Below we only consider the "reduced" distribution on position variables.)

The study of ground states for (infinite) systems of particles with positions on a fixed lattice was begun 30 years ago by Ruelle ([Ru]) and Schrader ([Sc]), including a simple characterization of the support of such states. However no analogous result was ever published for systems of particles with positions in $\mathbb{R}^n$. We provide this for the special case of strictly finite range interactions with hard core, and make some conjectures about the more difficult case without hard core.

2 Notation and Assumptions

Let U be some pair potential, which is translation and rotation invariant, i.e. $U(s,t) = U(|s-t|)$. We suppose U to be superstable. The Lennard-Jones potential is an example of such interaction. Let λ be some chemical potential.

Our initial modest goal was to prove that for all reasonable interactions U the following holds:

Statement. *Let $\beta_n \to \infty$ be a sequence of inverse temperatures, going to infinity, and let μ_n be a weakly converging sequence of Gibbs states, corresponding to the interaction U, chemical potential λ and inverse temperatures β_n, i.e. $\mu_n \in \mathcal{G}(U, \lambda, \beta_n)$. Then for sufficiently negative λ the limiting state μ_∞ is supported by the set G of ground state configurations.*

For every U, λ there exist a pair of constants $\underline{R} < \overline{R}$, such that for every

$\omega = \{\omega_k\} \in G$

$$\inf_{i<j} |\omega_i - \omega_j| > \underline{R}, \tag{1}$$

and every ball $B_r \subset R^n$ of radius $r > \overline{R}$ contains at least one particle $\omega_i \in \omega$.

If true, these properties would be a zero-level approximation to the ordered structure which is expected (in some sense) to be formed by solids.

We have to say that we do not expect the above picture to hold without extra assumptions, though these assumptions are expected to be mild and physically natural. But first we will formulate some conjectures which appear to us to be provable.

Let $\mu \in \mathcal{G}(U, \lambda, \beta)$ be some random point field with inverse temperature β. Denote by $\rho_\mu(x)$ the expected number of particles of the field μ in the unit ball centered at the point $x \in \mathbb{R}^n$.

Proposition 1 *For every λ, β and U without hard core there exists a state $\bar{\mu} \in \mathcal{G}(U, \lambda, \beta)$, such that the function $\rho_{\bar{\mu}}(\cdot)$ is unbounded on $\mathbb{R}^n$.*

That statement means that the relation (1) can not hold in general.

Proposition 2 *Suppose that the state $\tilde{\mu} \in \mathcal{G}(U, \lambda, \beta)$ has the density function $\rho_{\tilde{\mu}}(\cdot)$, which is polynomially bounded, i.e. there exists a polynomial $P(\cdot)$, such that $\rho_{\tilde{\mu}}(x) \leq P(x)$, $x \in \mathbb{R}^n$. Then there exists a constant $C = C(U, \lambda)$, such that $\rho_{\tilde{\mu}}(x) \leq C$.*

The proof of Proposition 2 can be obtained by the application of the technique of compact functions, developed by R. Dobrushin in ([D1]), see also ([D2]). Being proven, Proposition 2 can be used to deduce the existence of the constants $\underline{R}, \overline{R}$ above, under condition that the random fields we are dealing with all have their density functions polynomially bounded (and hence, uniformly bounded).

Proposition 1 can be derived from Proposition 2 and the following construction. We will consider the 1D case; the generalization to higher dimensions is obvious. Let us suppose that $r_1 < 1$, $r_2 > 2$. Let I_n be the unit segment centered at the integer point $n \in \mathbb{R}^1$. Let ϖ^{-1}, ϖ^1 be two configurations in the segments I_{-1}, I_1, and consider the conditional Gibbs distribution $q(\omega^0|\varpi^{-1}, \varpi^1)$ in I_0, given configuration $\varpi^{-1} \cup \varpi^1$ outside. Let $K > 0$ be fixed. Clearly, there exists a number $N(1)$, such that if $|\varpi^{-1}| > N(1)$,

$|\varpi^1| > N(1)$, then $2K > \mathbb{E}(|\omega^0|) > K$. Let now ϖ^{-2}, ϖ^2 be two configurations in the segments I_{-2}, I_2, and consider the conditional Gibbs distribution $q(\omega|\varpi^{-2}, \varpi^2)$ in $I_{-1} \cup I_0 \cup I_1$, given configuration $\varpi^{-2} \cup \varpi^2$ outside. Clearly, there exists a number $N(2)$, such that if $|\varpi^{-2}| > N(2)$, $|\varpi^2| > N(2)$, then $\mathbb{E}(|\omega^1|) > N(1)$, $\mathbb{E}(|\omega^{-1}|) > N(1)$, and so again $\mathbb{E}(|\omega^0|) > K$. Here we denote by ω^k the restriction of ω on the segment I_k. If the number $N(2)$ is not too big, then we have in addition that $\mathbb{E}(|\omega^0|) < 2K$. We can repeat this construction inductively in n. As a result, by taking a limit point we get an infinite volume Gibbs state on $\mathbb{R}^1$, such that $\mathbb{E}(|\omega^0|) > K$. If K is chosen large enough: $K > C(U, \lambda)$, then the so constructed state has the function $\rho(\cdot)$ unbounded, due to Proposition 2.

In what follows we present a proof of our Statement, restricted to the case of interaction with hard core. This assumption only plays a technical role, and with an extra effort we expect it can be removed.

3 Convergence to Ground State Configurations

First some notation and assumptions. We assume a two-body interaction $U(s,t)$ dependent only on the separation of the point particles at positions s, t in $\mathbb{R}^n$, with a hard core at separation 1, and diverging as the separation decreases to 1. We assume U has strictly finite range $R > 1$, and that $U \geq -m$, $m > 0$. Denote the chemical potential by λ. We only consider $\lambda \leq 0$.

We denote by Ω the set of all finite or countably infinite configurations $\omega \subset \mathbb{R}^n$ of particles which are separated by a distance at least 1. By ω_j we denote the positions of the particles in ω, and by $b_1(\omega)$ the set of balls $b_1(\omega_j)$ of diameter 1 centered at positions ω_j. For $A \subset \mathbb{R}^n$ we denote by Ω_A the set of configurations $\omega = \omega_A \equiv \omega \cap A$, which have all their particles in A. The number of particles in ω_A will be denoted by $|\omega_A|$.

With the usual topology Ω is compact. For $\beta > 0$ we denote by μ_β any Gibbs measure for our interaction at inverse temperature β. We note without proof that any such measure gives probability 1 to the set of configurations in which no two particles are at distance 1.

For every bounded A and $\omega \in \Omega_A$ we define the energy:

$$H(\omega) = \sum_{i<j} U(\omega_i, \omega_j) + \lambda |\omega| \,. \tag{2}$$

For two collections of particles, $\omega' \in \Omega_A$, $\omega'' \in \Omega$, we define the interaction between them as

$$H(\omega', \omega'') = \sum_{i,j} U(\omega'_i, \omega''_j). \tag{3}$$

and the sum

$$H(\omega'|\omega'') = H(\omega') + H(\omega', \omega''). \tag{4}$$

Let the set G of "ground state configurations" be defined as:

$$\begin{aligned} G = \{\omega \in \Omega :\ & \text{for every bounded } \Lambda \subset \mathbb{R}^n \text{ and every } \omega' = (\omega'_\Lambda, \omega_{\Lambda^c})\,, \\ & H(\omega'_\Lambda|\omega_{\Lambda^c}) - H\left(\omega_\Lambda|\omega_{\Lambda^c}\right) \geq 0\}, \end{aligned}$$

where Λ^c denotes the complement of Λ. We note without proof that G is compact.

Our main result is the following

Theorem 3 *The set G is nonempty. Let μ_∞ be any limit point of the family of Gibbs states μ_β as $\beta \to \infty$. Then $\mu_\infty(G) = 1$.*

(The fact that G is nonempty was proved somewhat more generally in ([Ra]).)

Our claim is equivalent to the

Theorem 4 *Assume that $\omega \in G^c$. Then there exists an open neighborhood W of ω such that $\int_W \, d\mu_\beta(\sigma) \to 0$ as $\beta \to \infty$.*

Proof. Before giving the formal proof we present its simple idea. If $\omega \in G^c$ then the following holds: there exists a finite volume B, inside which the configuration $\omega \equiv (\omega_B, \omega_{B^c})$ can be modified into $\bar\omega \equiv (\bar\omega_B, \omega_{B^c})$ in such a way that

$$\Delta(\omega) \equiv H\left(\omega_B|\omega_{B^c}\right) - H\left(\bar\omega_B|\omega_{B^c}\right) > 0. \tag{5}$$

We will be done if we can find *open* neighborhoods $W, \bar W$ of the configurations ω and $\bar\omega$ and show that

$$\frac{\mu_\beta(W)}{\mu_\beta\left(\bar W\right)} \to 0 \tag{6}$$

as $\beta \to \infty$. So we need to find an upper bound for $\mu_\beta(W)$ and a lower bound for $\mu_\beta(\bar{W})$. To do this we will use the following simple

Lemma 5 *For every value of the chemical potential $\lambda < 0$ there exists a distance $\rho(\lambda) > 1$ such that the following holds for all ρ in the interval $(1, \rho(\lambda))$:*

Let $M \subset \mathbb{R}^n$ be any bounded volume and $\xi \in \Omega_{M^c}$ – any "boundary condition". Denote by $\Omega_{M,\rho}(\xi) \subset \Omega_M$ the subset

$$\left\{ \begin{array}{c} \sigma \in \Omega_M : \textit{two particles of } \sigma \textit{ are separated by } < \rho, \textit{ or a particle of } \sigma \\ \textit{is at distance } < \rho \textit{ from a particle of } \xi \end{array} \right\}. \tag{7}$$

Then the conditional Gibbs probability

$$q_{M,T}(\Omega_{M,\rho}(\xi) | \xi) \tag{8}$$

goes to 0 as $T \to 0$. This convergence, of course, is not uniform in M, but for every M it is uniform in ξ. Therefore,

$$q_{M,T}(\Omega_M \setminus \Omega_{M,\rho}(\xi) | \xi) = q_{M,T}(\Omega_M | \xi)(1 - \gamma(T, M, \xi, \rho)), \tag{9}$$

where for every M, ρ the function $\gamma(T, M, \xi, \rho) \to 0$ as $T \to 0$, uniformly in ξ.

The same statement holds for the subset

$$\Omega_{M,\rho} = \{\sigma \in \Omega_M : \textit{two particles of } \sigma \textit{ are at distance } < \rho\}, \tag{10}$$

since for every ξ we have $\Omega_{M,\rho} \subset \Omega_{M,\rho}(\xi)$.

Without the hard core condition Lemma 5 does not hold, and would have to be replaced by a weaker statement. Our proof of Lemma 5 uses the divergence of the repulsion near the hard core.

The proof of Theorem 4 proceeds now as follows. Let $\bar{B}$ be the open R-neighborhood of B. Without loss of generality we can assume that $\omega \notin \Omega_{\bar{B},\rho(\lambda)}$.

By an r-perturbation of a finite configuration $\varpi \in \Omega$ we will mean any finite configuration $\varkappa$ with the same number of particles, such that for every particle $\varpi_j \in \varpi$ the intersection $\varkappa \cap b_1(\varpi_j)$ consists of precisely one particle $\varkappa_j \in \varkappa$, and $\mathrm{dist}(\varpi_j, \varkappa_j) < r$.

Now we define the open neighborhood W of ω by putting

$$W=\left\{ (\varkappa,\xi):\varkappa\in\Omega_{r}\left(\omega,\bar{B}\right),\xi\in\Omega_{\bar{B}^{c}}\right\} , \tag{11}$$

where $\Omega_{r}\left(\omega,\bar{B}\right)$ is the set of all those r-perturbations $\varkappa$ of $\omega_{\bar{B}}$ which also belong to $\Omega_{\bar{B}}$. It is easy to see that if $r\leq\rho(\lambda)/2$ then for every $(\varkappa,\xi)\in W$

$$\left|H\left(\varkappa_{B}\right)-H\left(\omega_{B}\right)\right|<Cr,$$
$$\left|H\left(\varkappa_{B},\varkappa_{\bar{B}\backslash B}\right)-H\left(\omega_{B},\omega_{\bar{B}\backslash B}\right)\right|<Cr,$$

for some $C=C\left(B\right).$ Let r be so small that $Cr<\frac{\Delta(\omega)}{10}$. Then, by DLR,

$$\begin{aligned}
&\int_{W}d\mu_{\beta}\left(\varkappa,\xi\right)\\
&=\int_{\Omega_{r}\left(\omega,\bar{B}\right)}\frac{1}{Z_{B}\left(\varkappa_{\bar{B}\backslash B}\right)}\left[\int_{\Omega_{r}\left(\omega,\varkappa_{\bar{B}\backslash B}\right)}\exp\left\{-\beta H\left(\varkappa_{B}|\varkappa_{\bar{B}\backslash B}\right)\right\}d\Pi_{B}(\varkappa_{B})\right]d\mu_{\beta}\left(\varkappa,\xi\right)\\
&\leq\exp\left\{-\beta\left[H\left(\omega_{B}|\omega_{B^{c}}\right)-\frac{\Delta\left(\omega\right)}{10}\right]\right\}\int_{\Omega_{r}\left(\omega,\bar{B}\right)}\frac{1}{Z_{B}\left(\varkappa_{\bar{B}\backslash B}\right)}d\mu_{\beta}\left(\varkappa,\xi\right),
\end{aligned}$$

where

$$\Omega_{r}\left(\omega,\varkappa_{\bar{B}\backslash B}\right)=\left\{\tilde{\varkappa}\in\Omega_{r}\left(\omega,\bar{B}\right):\tilde{\varkappa}_{\bar{B}\backslash B}=\varkappa_{\bar{B}\backslash B}\right\}, \tag{12}$$

Π_{B} denote the (free) Poisson measure in B with rate 1, and the $Z_{B}\left(\varkappa_{\bar{B}\backslash B}\right)$'s are the normalization constants (partition functions).

In the same way, and recalling the meaning of $\bar{\omega}$, we put

$$\bar{W}=\left\{(\varkappa,\xi):\varkappa\in\Omega_{r}\left(\bar{\omega},\bar{B}\right),\xi\in\Omega_{\bar{B}^{c}}\right\}. \tag{13}$$

Without loss of generality we can assume that for the same C and every $(\varkappa,\xi)\in\bar{W}$

$$\left|H\left(\varkappa_{B}\right)-H\left(\bar{\omega}_{B}\right)\right|<Cr,$$
$$\left|H\left(\varkappa_{B},\varkappa_{\bar{B}\backslash B}\right)-H\left(\bar{\omega}_{B},\omega_{\bar{B}\backslash B}\right)\right|<Cr.$$

Then

$$\begin{aligned}
&\int_{\bar{W}}d\mu_{\beta}\left(\varkappa,\xi\right)\\
&=\int_{\Omega_{r}\left(\omega,\bar{B}\right)}\frac{1}{Z_{V}\left(\varkappa_{\bar{B}\backslash B}\right)}\left[\int_{\Omega_{r}\left(\bar{\omega},\varkappa_{\bar{B}\backslash B}\right)}\exp\left\{-\beta H\left(\varkappa_{B}|\varkappa_{\bar{B}\backslash B}\right)\right\}d\Pi_{B}(\varkappa_{B})\right]d\mu_{\beta}\left(\varkappa,\xi\right)\\
&\geq\exp\left\{-\beta\left[H\left(\bar{\omega}_{B}|\omega_{B^{c}}\right)+\frac{\Delta\left(\omega\right)}{10}\right]\right\}\int_{\Omega_{r}\left(\omega,\bar{B}\right)}\frac{1}{Z_{V}\left(\varkappa_{\bar{B}\backslash B}\right)}\left[\int_{\Omega_{r}\left(\bar{\omega},\varkappa_{\bar{B}\backslash B}\right)}d\Pi_{B}(\varkappa_{B})\right]d\mu_{\beta}\left(\varkappa,\xi\right),
\end{aligned}$$

But the integral $\int_{\Omega_r\left(\bar{\omega},\varkappa_{\bar{B}\setminus B}\right)} d\Pi_B(\varkappa_B)$ is just the Poisson measure of the set $\Omega_r\left(\bar{\omega}\right)$, so it is a positive number (not depending on β). The comparison of the last two estimates proves our theorem. $\square$

Proof of the Lemma. After the above discussion it is straightforward. Let $i\left(n\right)$ be the maximal number of particles with which any given particle can interact. Suppose a particle ϖ_1 is ρ-close to ϖ_2. Then the interaction $U\left(\varpi_1,\varpi_2\right) > \lambda + i\left(n\right)m + 1$, provided $\rho - 1$ is small enough. But then if we erase the particle ϖ_1, we gain at least one unit of energy. The rest of the argument follows the same line as above. $\square$

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