EXISTENCE OF GROUND STATE CONFIGURATIONS

by

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Abstract

We prove the existence of energy ground state configurations for systems of infinitely many particles interacting, in d-dimensional space, through any of a wide class of finite range, many-body potentials with hard core.

February 2004

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* Research supported in part by NSF Grant No. DMS-0071643 and
Texas ARP Grant 003658-158

I. Introduction

We are concerned with systems of interacting particles in d-dimensional Euclidean space $\mathbb{E}^d$, $d \geq 1$, with particles of one or more species, in thermal equilibrium. We assume the interaction includes a hard core, which need not be spherically symmetric, so the system is perhaps better described as interacting molecules or bodies. We will assume given some Euclidean invariant interaction potential ϕ, which associates an energy $\phi(C)$, in $\mathbb{R} \cup +\infty$, to any finite collection $C \subset \mathbb{E}^d$ of at least two bodies, subject to the weak conditions listed in the next section.

We are interested in the *geometric symmetries* of solid thermodynamic phases, so we will work with infinite systems of particles, distributed throughout $\mathbb{E}^d$. There is a well developed formalism for describing such systems in a limiting grand canonical ensemble [Ru], [Pr], with parameters T for temperature, and chemical potentials μ_i for each species i of particle. It is common to (try to) approximate the low temperature distribution as a perturbation of "energy ground state configurations". This has been particularly successful in lattice gas models, in which the particles are centered on the vertices of some lattice or graph (see [G], [HP]), but it is controversial to what extent such models can reliably represent solids – especially to investigate geometric symmetries! Returning then to particles in a continuum, we note that there is no published model exhibiting even such a basic feature as the existence of a solid phase at $T > 0$, let alone any analysis of the symmetries of such solid phases. But we expect that in some cases of our continuum models, if $T > 0$ is small enough the distribution is concentrated on perturbations of configurations for which the total energy is everywhere minimized in some appropriate sense. Heuristically, such configurations x, spatially extended throughout $\mathbb{E}^d$, are supposed to minimize a global energy $H(x)$ which is a sum of contributions, one for each particle/body b in x, of amount

$$\hat{L}(x;b) = -\mu(b) + \sum_{C\subset x,\ C\ni b} \phi(C), \qquad 1)$$

where $\mu(b)$ is the chemical potential of b. There is no direct meaning to $H(x)$ since in interesting cases it is infinite; instead we will use the traditional criterion for energy ground state configurations based on a form of local optimality for all local regions.

To give a proper definition of energy ground state configurations we first need some notation. For each particle species i, of which there are $M \geq 1$, we assume given some body b_i, that is, a compact, connected set with dense interior and boundary of zero volume, representing the hard core for that species. We define X as the space of all possible packings of $\mathbb{E}^d$ by congruent copies of the bodies, with the usual metrizable topology in which two packings are close if, within a large ball around the origin of $\mathbb{E}^d$, the two packings are uniformly close (that is, close in the Hausdorff metric on compact sets) [Ra1]. X is compact in that topology. Assume given a cube $B \subset \mathbb{E}^d$, and two packings $x, y \in X$. Then: $V_i[B;(y,x)]$ will denote the total volume of the intersections $b \cap B$ of all those bodies b, of species i, such that either $b \in y$, or $b \in x$ and the interior of b intersects the boundary ∂B of B; $\bar{V}[B;(y,x)] = \{V_i[B;(y,x)]\}$; $\bar{\mu} = \{\mu_i\}$; and $\bar{\mu} \cdot \bar{V}[B;(y,x)] = \sum_i \mu_i V_i[B;(y,x)]$. A related but more complicated quantity is the local potential energy defined as follows, using the notation $v[A]$ to denote the volume, and $i(A)$ the interior, of $A \subset \mathbb{E}^d$:

$$\begin{aligned} E[B;(y,x)] = &\sum_{b \in y : b \subset B} \sum_{C \ni b} \phi(C) \\ &+ \sum_{b \in x : i(b) \cap \partial B \neq \emptyset} \frac{v[b \cap B]}{v[b]} \sum_{C' \ni b} \phi(C'). \end{aligned} \tag{2)}$$

We are now ready to define energy ground state configurations.

Definition 1. A configuration x is an energy ground state configuration (for given $\bar{\mu}$) if for *every* fixed cube $B \subset \mathbb{E}^d$

$$\inf_y \{E[B;(y,x)] - \bar{\mu} \cdot \bar{V}[B;(y,x)]\} = E[B;(x,x)] - \bar{\mu} \cdot \bar{V}[B;(x,x)]. \tag{3)}$$

This (traditional) criterion for a configuration x to be a minimizer for the global H is simply that it be locally stable: no change in x in a finite region can lower the contribution to $H(x)$ associated with that finite region. One consequence is that a minimizing configuration has the lowest possible energy density, as computed by averaging over an expanding sequence of regions.

The *existence* of such energy ground state configurations x is by no means obvious, and proof of their existence is our main result. (We compare this problem with the parallel one for lattice gas models in Section III.) If ϕ only takes the values $+\infty$ and 0 and the chemical potentials μ_i are taken to have special values (appropriate to the bodies b_i) this reduces to a result of Bowen [B] on completely saturated packings in $\mathbb{E}^d$.

II. Statement and Proof of Results

We assume our Euclidean invariant interaction potential ϕ satisfies the following general properties:

i) there is some R, larger than twice the diameter of any of the b_i, and $\phi(C) = 0$ if there is no ball of radius R containing all the bodies of C;
ii) $\phi(C) = +\infty$ if there is some ball of radius R containing all the bodies of C, and the interiors of some pair of bodies of C intersect;
iii) ϕ is continuous when restricted to the manifold of (positions and orientations of) packings of any given finite number, greater than 2, of bodies of given species, and on the manifold of packings of pairs of bodies of given species either: a) ϕ is continuous; or b) ϕ is bounded below and continuous on the subset of nontouching pairs, and $\phi(C) \to +\infty$ as the separation of the pair vanishes, and $\phi(C) = +\infty$ for touching pairs.

Our main result is the following.

Theorem 1. For any system of interacting particles/bodies with given interaction ϕ satisfying conditions i)–iii) and given chemical potentials $\bar{\mu}$ there exists a translation invariant probability measure $m_{_L}$, on the space X of possible packings of the bodies, for which a set of full measure consists of energy ground state configurations.

Proof of the theorem. First we define a function p on X by:

$$p(x) = \begin{cases} c(x), & \text{if the interior of a body } \tilde{b}(x) \text{ of } x \text{ contains } \mathcal{O} \\ 0, & \text{if no body of } x \text{ contains } \mathcal{O} \text{ in its interior} \end{cases} \tag{4)}$$

where $\mathcal{O}$ is the origin in $\mathbb{E}^d$ and $c(x) = 1/\text{volume}[\tilde{b}(x)]$. Then we define the function L on X, a density for $\hat{L}$ of 1), by

$$L(x) = p(x)\big[-\mu(x) + \sum_{C\subset x,\ C\ni b(x)} \phi(C)\big] \tag{5)}$$

where $b(x)$ is any body in x nearest to $\mathcal{O}$, and $\mu(x)$ is the chemical potential for that species of particle/body. (For completeness, in case one factor in 5) is 0 and the other is $+\infty$ we define the product to be 0, except in those cases where $\mathcal{O}$ is on a boundary of a body in x, in which case we define the product to be $+\infty$.) Note that the ambiguity of $b(x)$, and therefore of $\mu(x)$, is irrelevant to $L(x)$ because of the factor $p(x)$; $L(x)$ is nonzero only if some body b of x contains $\mathcal{O}$, and then represents the total energy of interaction of b with the rest of the bodies in x. Note that if $\chi_{_B}$ is the characteristic function for B

$$\int \chi_{_B}(g) L(x-g)\, dg = E[B;(x,x)] - \bar{\mu}\cdot \bar{V}[B;(x,x)]. \tag{6)}$$

Let $M(X)$ be the set of Borel probability measures on X in the weak-$*$ topology, which makes $M(X)$ compact, and let $M_I(X)$ be the subset of those measures which are invariant under the natural action of the translation group $\mathcal{G}^d(\approx \mathbb{R}^d)$ of $\mathbb{E}^d$. ($M_I(X)$ is easily seen to be a nonempty closed subset of $M(X)$.)

Lemma 1. There exists $m_{_L}$ in $M_I(X)$ such that $m_{_L}(L) = \inf\{m(L)\,|\, m \in M_I(X)\}$.

Proof of Lemma 1. We begin by smoothing a bit the function L. Define $\tilde{L}(x) = \sup\{f(x)\,|\, f \text{ continuous, and } f(y) \leq L(y), \text{ at all } y \in X\}$. It follows that $\tilde{L}$ is lower semicontinuous on X and bounded below. Thinking of Borel probability measures as functionals on the space of continuous functions on X, which one extends (with the possible value of $+\infty$) first to over functions and then integrable functions in the usual way [T], $\tilde{L}$ is an over function, and, as a function on $M(X)$, and therefore also $M_I(X)$, it is easy to see it is again lower semicontinuous. Therefore by compactness there is some $\tilde{m} \in M_I(X)$ such that $\tilde{m}(\tilde{L}) = \inf\{m(\tilde{L})\,|\, m \in M_I(X)\}$. We claim that $m(L) = m(\tilde{L})$ for all $m \in M_I(X)$. To see this we first note that L and $\tilde{L}$ only differ where L is not lower semicontinuous, and therefore only on the closed set of packings x such that the origin $\mathcal{O}$ lies on a boundary of a body in x. That this set has measure zero with respect to any $m \in M_I(X)$ follows easily by applying Birkhoff's pointwise ergodic theorem [W] to the characteristic function of that set of packings. This proves the claim, and we can then take $m_L = \tilde{m}$ to complete the proof of Lemma 1.

Let B_s, for $s > 0$, be the cube in $\mathbb{E}^d$ centered at $\mathcal{O}$ and with faces which are distance s from $\mathcal{O}$ and perpendicular to coordinate axes.

Lemma 2. For each $j \geq 1$ there exists a function $f_j : X \to X$ such that:

a) for every $x \in X$, every $v \in \mathbb{E}^d$ with integral coordinates, and with $B_{j,v}$ defined as $B_j - v(2j+R)$, we have $\inf_y \{E[B_{j,v};(y,x)] - \bar{\mu}\cdot\bar{V}[B_{j,v};(y,x)]\} = E[B_{j,v}; f_j(x), f_j(x)] - \bar{\mu}\cdot\bar{V}[B_{j,v}; f_j(x), f_j(x)]$;

b) f_j commutes with all translations $v(2j+R)$, $v \in \mathbb{E}^d$ having integral coordinates;

c) f_j is Borel measurable.

Proof of Lemma 2. Intuitively, what f_j will do to x is replace those bodies of x which are (fully) in any of the regions $B_{j,v}$ by a collection of bodies which minimizes the energy associated with that region, while leaving the other bodies of x as they were. Such an energy minimum exists for a given region because of the continuity of ϕ and V; the only difficulty therefore is to ensure conditions b) and c). We can ensure b) by simply choosing the replacement for each region by the same rule (in a sense that will be made clear below). It is harder to see how to ensure condition c). An example which illustrates the essence of our difficulty with condition c) is the one in 2-dimensions, with only one species of body, namely B_1, and ϕ consisting only of the hard core. Assume the chemical potential μ is positive, take the region $B = B_1$ and let x consist of the single body $B_1 + (2,0)$. The minimum of $E[B;(y,x)] - \bar{\mu}\cdot\bar{V}[B;(y,x)]$ is then $-\mu$, while for the translated packings $x - (\epsilon, 0)$ the minimum would be $-\epsilon\mu$ (for arbitrarily small $\epsilon > 0$). In other words, in choosing how to optimize the bodies in B the dependence on those not in B must be taken into account and condition c) requires that this be done measurably. This is a standard selection problem in optimization. From the lower semicontinuity of $E[B;(y,x)] - \bar{\mu}\cdot\bar{V}[B;(y,x)]$ as a function of $(y,x) \in X \times X$, and the obvious fact that the equation

$$\{(y,x) \mid E[B;(y,x)] - \bar{\mu}\cdot\bar{V}[B;(y,x)] = \inf_y E[B;(y,x)] - \bar{\mu}\cdot\bar{V}[B;(y,x)]\} \qquad 7)$$

is equivalent to

$$\{(y,x) \mid E[B;(y,x)] - \bar{\mu}\cdot\bar{V}[B;(y,x)] \leq \inf_y E[B;(y,x)] - \bar{\mu}\cdot\bar{V}[B;(y,x)]\}, \qquad 8)$$

it follows that for given x

$$\{y' \mid E[B;(y',x)] - \bar{\mu}\cdot\bar{V}[B;(y',x)] = \inf_y E[B;(y,x)] - \bar{\mu}\cdot\bar{V}[B;(y,x)]\} \qquad 9)$$

is closed. It then follows by the theorem of Kuratowski and Ryll-Nardzewski [Ro] that there exists a Borel measurable function (selection) $y = y(x)$ such that

$$E[B;(y(x),x)] - \bar{\mu}\cdot\bar{V}[y(x),x)] = \inf_y E[B;(y,x)] - \bar{\mu}\cdot\bar{V}[B;(y,x)]\}, \qquad 10)$$

which gives us condition c). This completes the proof of Lemma 2.

Returning to the proof of the theorem, for each $j \geq 1$ we define the measure $\tilde{m}_L^j$, on continuous functions h on X, by $\tilde{m}_L^j(h) = m_L(h \circ f_j)$ using the composition $(h \circ f_j)[x] = h[f_j(x)]$. We note that $\tilde{m}_L^j$ is invariant under the group $\mathcal{G}_j^d$ consisting of translations by $v(2j+R)$ for $v \in \mathbb{E}^d$ with integral coordinates: using the notation $h_g(x) = h(x-g)$, $\tilde{m}_L^j(h_g) = \tilde{m}_L(h_g \circ f_j) = m_L([h \circ (f_j)_g]) = m_L(h \circ f_j) = \tilde{m}_L^j(h)$ for $g \in \mathcal{G}_j^d$, where we used $(f_j)_g[x] = (f_j[x]) - g$ from b) to get the second equality and the invariance of m_L for the third. Now we define m_L^j by averaging $\tilde{m}_L^j$ over (the flat torus) B_j, which clearly makes m_L^j invariant under all of $\mathcal{G}^d$. We then have

$$\begin{aligned} m_L^j(L) &= \int \Big[\frac{\int \chi_{B_j}(g) L_g(x)\, dg}{\int \chi_{B_j}(g)\, dg}\Big]\, d\tilde{m}_L^j(x) \\ &= \int \Big[\frac{\int \chi_{B_j}(g) (L_g \circ f_j)(x)\, dg}{\int \chi_{B_j}(g)\, dg}\Big]\, dm_L(x). \end{aligned} \qquad 11)$$

Let $U_{j,n}$ be the set of packings x for which

$$\inf_y \{E[B_j;(y,x)] - \bar{\mu}\cdot \bar{V}[B_j;(y,x)]\} \leq E[B_j;(x,x)] - \bar{\mu}\cdot \bar{V}[B_j;(x,x)] - \frac{1}{n}. \qquad 12)$$

Then

$$\begin{aligned} m_L^j(L) &= \int \Big[\frac{\int \chi_{B_j}(g) (L_g \circ f_j)(x)\, dg}{\int \chi_{B_j}(g)\, dg}\Big] \chi_{U_{j,n}}(x)\, dm_L(x) \\ &\quad + \int \Big[\frac{\int \chi_{B_j}(g) (L_g \circ f_j)(x)\, dg}{\int \chi_{B_j}(g)\, dg}\Big] \chi_{U_{j,n}^c}(x)\, dm_L(x) \\ &\leq \int \Big[\frac{\int \chi_{B_j}(g) L_g(x)\, dg}{\int \chi_{B_j}(g)\, dg} - \frac{1}{n}\Big] \chi_{U_{j,n}}(x)\, dm_L(x) \\ &\quad + \int \Big[\frac{\int \chi_{B_j}(g) (L_g \circ f_j)(x)\, dg}{\int \chi_{B_j}(g)\, dg}\Big] \chi_{U_{j,n}^c}(x)\, dm_L(x) \\ &\leq m_L(L) - \frac{1}{n} m_L(\chi_{U_{j,n}}). \end{aligned} \qquad 13)$$

Therefore from the optimum property of m_L it follows that $m_L(\chi_{U_{j,n}}) = 0$. But then $m_L(\chi_U) = 0$ for $U = \cup_{j,n} U_{j,n}$, the set of configurations which are not energy ground states. ■

III. Summary

In lattice gas models the sets S_j, of configurations satisfying energy minimization with respect to the cubes B_j, are compact, nonempty, and decreasing as j increases, and therefore have a nonempty intersection. This is the structure of the simple proof for the existence of ground state configurations in lattice gas models

[S]. However such sets S_j are not compact in our continuum models as is made clear by the 2-dimensional example in the proof of Lemma 2. Instead (following Bowen [B]), we get existence of energy ground state configurations as the countable intersection of sets which are of full measure for $m_{_L}$. While it would seem more natural to work with a zero temperature limit measure instead of $m_{_L}$, this does not seem easy; on the contrary, perhaps $m_{_L}$ will find other uses.

The primary motivation of this paper is the analysis of the symmetry of low temperature matter, often analyzed as a perturbation of the energy ground state. Since the discovery of quasicrystals it has been necessary to look within a broader setting than the crystallographic groups for a general understanding of the geometric symmetry of solids [Ra1]-[Ra4], [BHRS]. Coupled with this is the tantalizing, but unsatisfactory, well-known argument [Pi] to explain the experimental nonexistence of a critical point separating the solid and fluid phases of matter, based on a supposed geometric symmetry for solids. There are indeed many ways in which the symmetry of energy ground state configurations are significant, for which the above existence theorem should be a useful step.

Acknowledgments. It is a pleasure to thank Klaus Bichteler and Charles Holton for useful discussions.

IV. References

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