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The Superstability of Pair-Potentials of Positive Type

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We prove that a pair-potential which is continuous, L^1, and of positive type satisfies a condition of the superstability kind with best-possible constants. The applications to statistical thermodynamics are mentioned.

KEY WORDS: Superstability; pair-potential; functions of positive type; thermodynamic limit.

1. INTRODUCTION

Following Ginibre,[1] we say that $\phi : \mathbb{R}^k \rightarrow \mathbb{R}$ is *superstable* if there exists a pair of constants, $A > 0$ and $B \geqslant 0$, such that for each finite set $\{x_1, x_2, \ldots, x_n\}$ of n distinct points of $\mathbb{R}^k$ the following inequality holds:

$$\sum_{i<j} \phi(x_i - x_j) \geqslant -Bn + An^2\Big(\max_{i,j}|x_i - x_j|\Big)^{-k} \tag{1.1}$$

Superstable pair potentials are important in the statistical thermodynamics of continuous systems (see Refs. 1 and 2, for example). In these applications use is made of the following simple consequence of (1.1):

Superstability Property. Suppose that ϕ is superstable and that Λ is an open subset of $\mathbb{R}^k$; then there exists a pair of constants $A_\Lambda > 0$, and $B \geqslant 0$, such that for each finite set $\{x_1, x_2, \ldots, x_n\}$ of n distinct points of Λ the following inequality holds:

$$\sum_{i<j} \phi(x_i - x_j) \geqslant -Bn + A_\Lambda n^2/\mathrm{vol}(\Lambda) \tag{1.2}$$

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The constant A_Λ is volume independent for a given shape, but may be shape dependent.

In establishing the superstability property for a given function the following criterion, due to Ruelle,[2] is often useful:

Ruelle's Criterion. Suppose that $\phi : \mathbb{R}^k \to \mathbb{R}$ satisfies the condition (R): ϕ is a continuous L^1 function of positive type; then ϕ is superstable if

$$\hat{\phi}(0) = \int_{\mathbb{R}^k} \phi(x)\, dx$$

is strictly positive.

Our aim in this paper is to prove a result along the lines of (1.2) for a function satisfying Ruelle's criterion, but with best-possible constants. The point of this is to provide us with a tool for proving the existence of limits by sandwiching a function between bounds which become equal in the thermodynamic limit. In order to get best-possible constants we have to be able to control the shape dependence. Following Fisher,[3] we define the shape factor $\sigma(\Lambda, h)$ for each $h > 0$ and each open set Λ by

$$\sigma(\Lambda, h) = \mathrm{vol}(\Lambda^h \backslash \Lambda)/\mathrm{vol}(\Lambda) \tag{1.3}$$

where

$$\Lambda^h = \{x : d(x, \Lambda) < h\} \quad \text{and} \quad d(x, \Lambda) = \inf_{y \in \Lambda} |x - y|$$

2. STATEMENT OF RESULTS

We state our first result as a lemma:

Lemma. Let $\phi : \mathbb{R}^k \to \mathbb{R}$ satisfy condition (R); then for each $h > 0$, each open set Λ of R^k, and each finite set of n distinct points of Λ, the following inequality holds:

$$\sum_{1 \leqslant i,j \leqslant n} \phi(x_i - x_j) \geqslant \frac{n^2}{\mathrm{vol}(\Lambda)} \frac{[\hat{\phi}(0) - \delta(h)]^2}{[\hat{\phi}(0) + \delta(h) + \sigma(\Lambda, h)\|\phi\|_1]} \tag{2.1}$$

where

$$\delta(h) = 2\int_{|x| > h} |\phi(x)|\, dx$$

In applications of the Lemma in statistical thermodynamics we deal with a sequence of sets whose shape factors converge to zero; such sequences were introduced in Ref. 3. A sequence $\{\Lambda_l : l = 1, 2, \ldots\}$ of open subsets of $\mathbb{R}^k$ is said to satisfy condition (F) if (F1) and (F2) hold:

(F1) For each $h > 0$ we have $\lim_{l\to\infty}\sigma(\Lambda_l, h) = 0$.

(F2) For each $R > 0$ there is an integer $l(R)$ such that $B(R) \subset \Lambda_l$ for all $l > l(R)$, where $B(R) = \{x : |x| \leqslant R\}$.

The following Theorem is an easy consequence of the Lemma:

Theorem. Let $\{\Lambda_l : l = 1, 2, \ldots\}$ be a sequence of open subsets of $\mathbb{R}^k$ satisfying condition (F); let $\phi : \mathbb{R}^k \to \mathbb{R}$ be a function satisfying condition (R) and such that $\hat{\phi}(0) > 0$. Then, given $\epsilon > 0$, there exists an integer $l(\epsilon)$ such that, for each finite set $\{x_1, \ldots, x_n\}$ of n distinct points of Λ_l, the following inequality holds:

$$\sum_{i<j} \phi(x_i - x_j) \geqslant -\frac{1}{2}\phi(0)n + \frac{1}{2}\left[(\hat{\phi}(0) - \epsilon)n^2\right]/\mathrm{vol}(\Lambda_l) \tag{2.2}$$

The constants $\phi(0)$ and $\hat{\phi}(0)$ in (2.2) are best possible.

It has been known for some time that a result of this kind must be true under suitable conditions. Lieb[4] sketched a proof and used the result to obtain the high-density limit of the ground-state energy per particle for an imperfect Bose gas; see also Ref. 5. Ruelle[2] gave a detailed proof, but his estimates resulted in a loss of best-possible constants. We have used the above theorem in Ref. 6 to prove the persistence of condensation in the van der Waals limit of an interacting boson gas. Conlon[7] has used it to prove that the ground-state energy per particle of a classical gas in the thermodynamic limit at high density ρ is $\frac{1}{2}\rho\hat{\phi}(0) - \frac{1}{2}\phi(0)$.

3. PROOF OF THE LEMMA

Recall the following result about functions of positive type (see Dixmier,[8] for example):

Proposition. For a continuous function $\phi : \mathbb{R} \xrightarrow{k} \mathbb{R}$ the following are equivalent:

(P1) ϕ is of positive type.

(P2) ϕ is bounded, and for each bounded measure μ on R^k:

$$\int\int \phi(x - y)\, \mu(dx)\, \mu(dy) \geqslant 0$$

Recall also that

If ϕ is of positive type then $\phi(-x) = \phi(x)$ and $|\phi(x)| < \phi(0)$.

From (P2) it follows that if ϕ is continuous and of positive type then it defines a positive-definite quadratic form

$$\langle \mu, \nu \rangle_\phi = \int\int \phi(x - y)\, \mu(dx)\, \nu(dy)$$

on the linear space of bounded measures on $\mathbb{R}^k$, so that the Cauchy–Schwartz inequality holds:

$$|\langle \mu, \nu\rangle_\phi|^2 \leqslant \langle \mu, \mu\rangle_\phi \langle \nu, \nu\rangle_\phi \tag{3.1}$$

Applying (3.1) with $\mu(dx) = \chi_{\Lambda^h}(x)\,dx$ and $\nu(dx) = \sum_{i=1}^n \delta_{x_i}(dx)$, where χ_{Λ^h} is the indicator function of the set Λ^h and δ_x is the Dirac measure concentrated at the point x, we have

$$\sum_{i,j} \phi(x_i - x_j) \geqslant \left| \sum_{i=1}^n A_\Lambda^h(x_i) \right|^2 \Big/ B_\Lambda^h \tag{3.2}$$

with

$$A_\Lambda^h(y) = \int_{\Lambda^h} \phi(x-y)\,dx \quad \text{and} \quad B_\Lambda^h = \int_{\Lambda^h} A_\Lambda^h(y)\,dy$$

Then

$$|A_\Lambda^h(y) - \hat{\phi}(0)| \leqslant \left| A_\Lambda^h(y) - \int_{B(h)} \phi(x)\,dx \right| + \frac{1}{2}\delta(h) \tag{3.3}$$

But around each point y of Λ there is a ball of radius h lying inside Λ^h, so that for each y in Λ we have

$$\left| A_\Lambda^h(y) - \int_{B(h)} \phi(x)\,dx \right| = \left| \int_{(\Lambda^h - y)\cap\{x\,:\,|x|>h\}} \phi(x)\,dx \right| \leqslant \frac{1}{2}\delta(h) \tag{3.4}$$

hence

$$|A_\Lambda^h(y) - \hat{\phi}(0)| \leqslant \delta(h) \tag{3.5}$$

for all y in Λ. Now

$$\begin{aligned} |B_\Lambda^h - \mathrm{vol}(\Lambda)\hat{\phi}(0)| &\leqslant \left| B_\Lambda^h - \int_{\Lambda^h}\int_\Lambda \phi(x-y)\,dx\,dy \right| + \left| \int_\Lambda A_\Lambda^h(y)\,dy - \hat{\phi}(0)\int_\Lambda dy \right| \\ &= \left| \int_{\Lambda^h}\int_{\Lambda^h\setminus\Lambda} \phi(x-y)\,dx\,dy \right| + \delta(h)\mathrm{vol}(\Lambda) \\ &\leqslant \int_{\mathbb{R}^k}\int_{\Lambda^h\setminus\Lambda} |\phi(x-y)|\,dx\,dy + \delta(h)\mathrm{vol}(\Lambda) \\ &= \|\phi\|_1 \mathrm{vol}(\Lambda^h\setminus\Lambda) + \delta(h)\mathrm{vol}(\Lambda) \end{aligned} \tag{3.6}$$

Using (3.4) and (3.6) in (3.2) we get (2.1).

4. PROOF OF THE THEOREM

It follows from the Lemma that if $\hat{\phi}(0) > 0$ then

$$\sum_{i,j} \phi(x_i - x_j) \geqslant \frac{n^2}{\mathrm{vol}(\Lambda)} \left[\hat{\phi}(0) - 3\delta(h) - \sigma(\Lambda, h)\|\phi\|_1 \right]$$

Since ϕ is in $L^1(R^k)$ we can choose h so that $\delta(h) < \epsilon/4$; since $\{\Lambda_l : l = 1, 2, \ldots\}$ satisfies condition (F) we can choose $l(\epsilon)$ such that $\sigma(\Lambda_l, h)\|\phi\|_1 < \epsilon/4$ for all $l > l(\epsilon)$. This establishes (2.2).

Suppose now that there is a sequence $\{A_l : l = 1, 2, \ldots\}$ of positive constants converging to $A > \hat{\phi}(0)$ and such that

$$\sum_{i,j} \phi(x_i - x_j) \geqslant \frac{n^2}{\mathrm{vol}(\Lambda_l)} A_l \tag{4.1}$$

for each finite set $\{x_1, \ldots, x_n\}$ of n distinct points of Λ_l. Then we can choose $\epsilon > 0$ such that $A - \epsilon > \hat{\phi}(0)$. Integrating both sides of (4.1) over Λ^n we have

$$\begin{aligned} n\phi(0) &+ \frac{n(n-1)}{\mathrm{vol}(\Lambda_l)} \left[\hat{\phi}(0) + \epsilon/2\right] \\ &\geqslant \left[\mathrm{vol}(\Lambda_l)\right]^{-n} \int_{\Lambda^n} \cdots \int \left\{ \sum_{i,j} \phi(x_i - x_j) \right\} dx_1 \ldots dx_n \\ &\geqslant \frac{n^2}{\mathrm{vol}(\Lambda_l)} (A - \epsilon/2) \end{aligned}$$

for l sufficiently large. Letting $n \to \infty$ we have $A - \epsilon < \hat{\phi}(0)$, contradicting the hypothesis. The optimality of $\phi(0)$ is now clear.

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