Equilibrium Distributions of Physical Clusters

Michael G. Mürmann
Institut für Angewandte Mathematik, Universität Heidelberg,
D-6900 Heidelberg, Federal Republic of Germany

Abstract. We consider classical systems of particles in \( \mathbb{R}^d \) interacting by a stable pair potential with finite range. We are engaged in subdividing every particle configuration into clusters of interacting particles and studying the cluster distributions corresponding to equilibrium particle distributions.

Introduction

Let us consider an interaction in the \( d \)-dimensional Euclidean space \( \mathbb{R}^d \) given by a pair potential \( \Phi \), i.e., the potential energy of particles located at \( x_1, \ldots, x_n \in \mathbb{R}^d \) is given by

\[ V(x_1, \ldots, x_n) = \sum_{1 \leq i < j \leq n} \Phi(x_j - x_i), \]

where \( \Phi: \mathbb{R}^d \to \mathbb{R} \cup \{ +\infty \} \) is Lebesgue measurable with \( \Phi(x) = \Phi(-x) \) for \( x \in \mathbb{R}^d \). We suppose \( \Phi \) to have the following properties:

- stability: there exists \( B \geq 0 \) with \( V(x_1, \ldots, x_n) \geq -nB \) for all \( n \) and \( x_1, \ldots, x_n \in \mathbb{R}^d \);
- finite range: there exists \( R > 0 \) with \( \Phi(x) = 0 \) for \( |x| > R \).

Because of the finite range property it is reasonable to introduce clusters of interacting particles. Thus a configuration \( (x_1, \ldots, x_i) \) is a cluster, iff each two particles of the cluster interact at least indirectly.

This is a special type of physical clusters introduced in 1939 independently by Frenkel and Band in order to discuss condensation phenomena (see [3]). Recently Sinai [8] defined similar clusters – clusters in space-time however – for the existence of the time evolution of particle configurations.

Every finite or infinite particle configuration can now be subdivided into clusters with possibly infinite clusters defined in the same way. The purpose of this paper is to study the distribution of cluster configurations corresponding to equilibrium particle distributions in the sense of the DLR-equations in the case of only finite clusters with probability 1.

In Section 1 we give the exact definition of clusters by means of cluster functions and denote relations of these functions describing the subdivision of finite particle configurations into clusters. These relations are used in Section 2 to derive the cluster distribution corresponding to a grand canonical particle
distribution of a bounded region. The result is a distribution, formally the same as a grand canonical distribution, if one introduces a certain measure on the cluster space and a hard core potential forbidding overlapping cluster configurations.

Section 3 treats the case of equilibrium particle distributions in $\mathbb{R}^d$. We give sufficient conditions for the absence of infinite clusters with probability 1, the essential condition being a low activity condition. In this case we show that the validity of the DLR-equations of the particle distribution is equivalent to cluster-DLR-equations of the corresponding cluster distributions with the above-mentioned measure and hard core potential.

In Section 4 we reverse the point of view and start from cluster configurations. We prove an existence theorem of cluster distributions satisfying the cluster-DLR-equations under the low activity condition. As a corollary we get an existence theorem of the corresponding particle distributions. Remark that concerning the behaviour of the potential for small distances it only presumes stability. We close in Section 5 with some remarks concerning the connection between the uniqueness of the equilibrium distribution and the absence of infinite clusters.

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1. Physical Clusters

The notion of clusters initiated in the introduction is equivalent to saying that a particle configuration is a cluster iff the graph obtained by joining interacting particles is connected. We use this fact to derive an explicit expression for a cluster function $u$ defined on all finite non-empty configurations, which is 1 for clusters and 0 otherwise.

For $x, y \in \mathbb{R}^d$ we set

$$h(x, y) = \begin{cases} 1 & \text{for } |x - y| > R \\ 0 & \text{for } |x - y| \leq R \end{cases}$$

and for $x_1, \ldots, x_n, y_1, \ldots, y_m \in \mathbb{R}^d$

$$h(x_1, \ldots, x_n; y_1, \ldots, y_m) = \prod_{i=1}^n \prod_{j=1}^m h(x_i, y_j).$$

This function is the usual function $h$ as defined in the theory of the Mayer expansion ([2]) related to the pair potential $\varphi$ given by:

$$\varphi(x) = \begin{cases} 0 & \text{for } |x| > R \\ +\infty & \text{for } |x| \leq R. \end{cases}$$

The cluster function $u$ is now defined on the topological sum $\sum_{l=1}^{\infty} (\mathbb{R}^d)^l$ representing the space of all finite non-empty configurations in the following way:

$$u(x_1, \ldots, x_l) = \sum_{G \in C_l} \prod_{(i,j) \in G} (1 - h(x_i, x_j)) \prod_{(a,b) \in G} h(x_a, x_b),$$

(1)

where $C_l$ is the set of all connected graphs $G$ with vertices $1, \ldots, l$. 