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Kinetic theory of cluster dynamics

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HIGHLIGHTS

- Cluster dynamics is formulated within the kinetic theory of Boltzmann.
- A macroscopic fraction of the gas forms a giant cluster in finite time.
- Critical index agrees with experimental results on the elastic billiard.

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ABSTRACT

In a Newtonian system with localized interactions the whole set of particles is naturally decomposed into dynamical clusters, defined as finite groups of particles having an influence on each other's trajectory during a given interval of time. For an ideal gas with short-range intermolecular force, we provide a description of the cluster size distribution in terms of the reduced Boltzmann density. In the simplified context of Maxwell molecules, we show that a macroscopic fraction of the gas forms a giant component in finite kinetic time. The critical index of this phase transition is in agreement with previous numerical results on the elastic billiard.

1. Introduction

As a proposal to gain insight on the statistical properties of large systems in a gaseous phase, N. Bogolyubov suggested to investigate a simple notion of *cluster decomposition* characterizing the collisional dynamics [1]. When the evolution is determined by a sequence of single, distinct, two-body interactions, a natural partition of the system can be defined in terms of *groups* of particles connected by a chain of collisions, so that a "cluster" consists of elements having affected each other's trajectory.

This notion has been developed later on, in connection with the problem of the Hamiltonian dynamics of an infinite system. In a Newtonian system, particles with rapidly increasing energies at infinity may generate instantaneous collapses for special initial configurations [2]. Mathematically, one needs to prove that such initial data form a set of measure zero in the phase space of infinitely many particles. In fact, one possible strategy to construct the dynamics is to show that, at properly fixed time, the system splits up into an infinite number of clusters which are moving *independently* as finite-dimensional dynamical systems. After some random interval of time, the partition into independent clusters changes, and one iterates the procedure. This dynamics is known as *cluster dynamics* and its existence has been proved first in [3] for some one-dimensional models (see [4] for generalizations).

In more recent years, the statistical properties of cluster dynamics of a system obeying Newton's law have been studied numerically [5]. In this reference, the authors focus on the frictionless elastic billiard in a square two-dimensional box with reflecting walls, and show that the dynamics undergoes a phase transition. This occurs in a way reminiscent of problems in percolation theory. Namely, the maximal (largest) cluster starts to increase dramatically at some critical time. At the critical time, the fraction of mass in the maximal cluster is rather small ($\sim$7% for 5000 disks at small volume density). After the critical time, it approaches the total mass of the system with exponential rate. Moreover, the transition is distinguished by a power-law behaviour for the cluster size distribution with exponent 5/2. Such critical index is believed to be *universal*, since it has been observed for several different models (see also [6]).

The cluster dynamics concept, together with the above described statistical behaviour, appear as well in a number of

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applied papers, e.g. geophysics, economics, plasma physics: see [5] and references therein.

Kinetic theory often provides successful methods for the computation of microscopic quantities related to properties of the dynamical system, for instance Lyapunov exponents or Kolmogorov–Sinai entropies [7–10]. In the present work, we are concerned with the cluster dynamics of an ideal gas where the kinetic description of Boltzmann based on molecular chaos applies.

Our setting is given by a density function $f = f(x, v, t)$ describing the amount of molecules having position $x \in \Lambda \subset \mathbb{R}^d$ and velocity $v \in \mathbb{R}^d$ at time t, and evolution ruled by

$$(\partial_t + v \cdot \nabla_x) f = \int_{\mathbb{R}^d \times S^{d-1}} dv_1 d\omega\, B(v - v_1, \omega) \left\{ f' f_1' - f f_1 \right\}, \tag{1.1}$$

where $f = f(x, v, t), f_1 = f(x, v_1, t), f' = f(x, v', t), f_1' = f(x, v_1', t)$, (v, v_1) is a pair of velocities in incoming collision configuration and (v', v_1') is the corresponding pair of outgoing velocities when the scattering vector is ω:

$$\begin{cases} v' = v - \omega[\omega \cdot (v - v_1)] \\ v_1' = v_1 + \omega[\omega \cdot (v - v_1)]. \end{cases} \tag{1.2}$$

The time-zero density $f(x, v, 0) = f_0(x, v)$ is fixed. For simplicity, the gas moves in the square d-dimensional box Λ of volume 1, with reflecting boundary conditions. The microscopic potential is assumed to be short-ranged and the cross-section B satisfies $\int d\omega B(v - v_1, \omega) = a(|v - v_1|) < \infty$ ("Grad's cut-off assumption").

The precise connection with a dynamical system of N particles interacting at mutual distance ε, such as the one studied in [5], can be established locally in the low-density limit

$$N \to \infty, \quad N\varepsilon^{d-1} \simeq 1, \tag{1.3}$$

("Boltzmann–Grad regime") as the convergence of correlation functions to the solution of the Boltzmann equation [11] (see also [12,10,13–15]). In the regime (1.3), the gas is so dilute that only two-body collisions are relevant. Furthermore, the collisions are completely localized in space and time. The limit transition (1.3) explains the microscopic origin of irreversible behaviour [16].

Our purpose here is to describe how the cluster size distribution is constructed from the solution to the Boltzmann equation. This is done in Section 2 by means of a suitable tree graph expansion, which is inspired by previously known formulas representing the Boltzmann density as a sum over collision sequences [17]. In Section 3, we indicate how to derive formally the introduced expressions as the limiting cluster distributions of a system of hard spheres in the Boltzmann–Grad scaling. Finally, in Section 4, we restrict to the simplest nontrivial (and paradigmatic) case in kinetic theory, i.e. the model of Maxwellian molecules. We show that the cluster distribution exhibits a phase transition characterized by a breakdown of the normalization condition at finite time. This implies that the "percolation" *survives* in the Boltzmann–Grad limit, with same qualitative behaviour and same critical index of the elastic billiard analysed in [5].

2. Cluster distributions

2.1. Bogolyubov clusters

We start with a formal notion of cluster. Let t be a given positive time.

Definition 1. (i) Two particles are t-neighbours if they collided during the time interval $[0, t]$.
(ii) A Bogolyubov t-cluster is any connected component of the neighbour relation (i).

The definition can be generalized to generic time intervals $[s, s+t]$. However, in what follows we will study the notion of t-cluster only, which is no restriction, and drop often the t-dependence in the nomenclature.

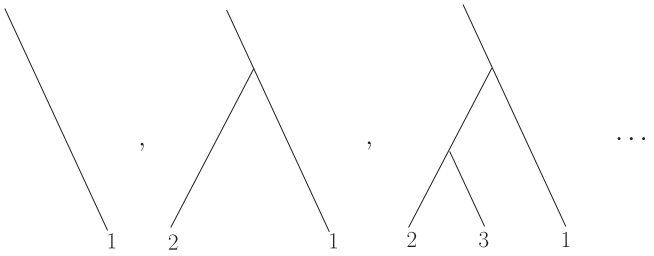
Notice that each particle has collided with *at least* one other particle of its Bogolyubov cluster, while it has *never* collided with particles outside the cluster, within the time interval $[0, t]$. In particular, if $t = 0$, *any* particle of the gas forms a singleton (cluster of size 1). At $t > 0$, the mass of singletons starts to decrease and clusters of size $k = 2, 3, \ldots$ start to appear. We therefore expect to see (and do observe in the experiments) some "smooth" exponential distribution in the cluster size.

2.2. Backward clusters

In Ref. [18], the solution of (1.1) has been expanded in terms of a sum of type

$$f = \sum_{n=0}^{\infty} \sum_{\Gamma_n} f^{\Gamma_n}, \tag{2.1}$$

where $\Gamma_0 = \emptyset$, $\Gamma_n = (k_1, k_2, \ldots, k_n)$ and $k_1 \in \{1\}, k_2 \in \{1, 2\}, \ldots, k_n \in \{1, 2, \ldots, n\}$. The sequences Γ_n are in one-to-one correspondence with binary tree graphs, e.g.



(2.2)

for $n = 1, 2, 3, \ldots$, respectively. In (2.1), f^{Γ_n} is interpreted as the contribution to the probability density f due to the event: *the backward cluster of* 1 *has structure* Γ_n. By "backward cluster" we mean here the group of particles involved directly or indirectly in the backwards-in-time dynamics of particle 1. Operatively, in a numerical experiment, we select particle 1 at time t, run the system backwards in time, and collect all the particles which collide with 1 and with "descendants" of 1 in the backwards dynamics, following (2.2). In other words, (2.1) is an expansion on sequences of real collisions.[1]

Formulas of this kind have been previously studied in the context of Maxwellian molecules with cut-off under the name of Wild sums [17,19,20], and are written in [18] for a gas of hard spheres in a homogeneous state. It is not difficult to generalize such a representation to inhomogeneous states and general interactions. The formula for f^{Γ_n} reads

$$\begin{aligned} f^{\Gamma_n}(x_1, v_1, t) = & \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \\ & \times \int_{\mathbb{R}^{nd}} dv_2 \cdots dv_{1+n} e^{-\int_{t_1}^t ds R_1(\zeta_1(s), s)} \\ & \times \left(\prod_{r=1}^{n} \int_{S^{d-1}} d\omega_r B(\eta_{k_r}^{r-1} - v_{1+r}, \omega_r) \right. \end{aligned}$$

[1] Observe that recollisions (e.g. the pair (1,2) colliding twice in the backward history), certainly possible in an experiment, do not affect the notion of backward cluster, which is based on sequences of collisions involving at least one "new" particle; see [18] for details on the numerical procedure.