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ON THE COLLISION RATE IN THE HARD DISK FLUID

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Abstract: N hard disks are injected into a 2-dimensional container. The initial velocities of the disks are generated according to a centered normal distribution. The Newtonian dynamics is imposed on the thermodynamic system (fluid). The collision rate of the disks is estimated from computer experimental data. A semi-empirical formula for the collision rate as a function of thermodynamic fluid parameters is proposed. This formula turns out to be valid for a wide range of fluid densities.

AMS Subject Classification: 82B30
Key Words: molecular dynamics, Boltzmann system, computer experiment

1. Introduction

An important and conceptually simple microscopic model for a substance is the Boltzmann system of moving molecules that are described by hard spheres, or, in the 2-dimensional case, by hard disks. In this model the molecules are subject to (thermal) motion and interact through collisions. In the context of microscopic explanation of reaction-kinetic phenomena one is interested in the collision process, in particular in the collision rate.

For the dilute range of the density of the fluid, kinematic considerations entail a theoretical formula for the collision rate. The aim of the present contribution is the computer experimental exploration of the quality of the formula

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and its correction which turns out to be valid for the whole range $0 < \varrho_r < 1$ of relative fluid density ϱ_r.

2. The Arrangement and the Outcome of the Computer Experiment

Let us consider a rectangular container

$$C := [-a_1, a_1] \times [-a_2, a_2] \subset \mathbb{R}^2,$$

where

$$a_2 = \frac{\sqrt{3}}{2} \cdot a_1. \tag{2.1}$$

We inject $N = 1827$ hard disks of mass $m = N_A^{-1}$ and radius $r = 10^{-10}$m into C where $N_A = 6.022 \cdot 10^{26}\text{kg}^{-1}$ denotes the modified Avogadro number.

We generate the initial velocities of the disks according to the normal distribution $N(0, \sigma^2 \cdot I_2)$ with mean vector $0 \in \mathbb{R}^2$ an covariance matrix $\sigma^2 \cdot I_2$ where I_2 denotes the 2×2 - identity matrix. This initial state complies with Maxwell hypothesis, cf. [3].

In all computer experiments reported in the present contribution parameter σ has been fixed:

$$\sigma := 1.$$

Newtonian dynamics has been imposed on the system of N disks confined to container C enabling us to determine positions $x^{(1)}(t), \dots, x^{(N)}(t) \in C$ and velocities $v^{(1)}(t), \dots, v^{(N)}(t) \in \mathbb{R}^2$ of the disks at any time $t \geq 0$.

During the temporal evolution of the microstate of the system (fluid) the disks collide with each other and we are interested in the collision rate λ. If the collisions between the disks are counted in the time interval $[0, \tau]$, then

$$\widehat{\lambda}(\tau) = \frac{c(\tau)}{\tau} \qquad (\tau \text{ large}) \tag{2.2}$$

is a natural estimator of λ where $c(\tau)$ denotes the number of collisions observed in the time interval $[0, \tau]$.

The computer experiment has been repeated 300 times where the relative density

$$\varrho_r = 2\sqrt{3} \cdot r^2 \cdot \frac{N}{V}$$

has been varied within the interval $(0, 1)$ by imposing appropriate volumes V of container C.

At every repetition of the experiment the collision process has been observed

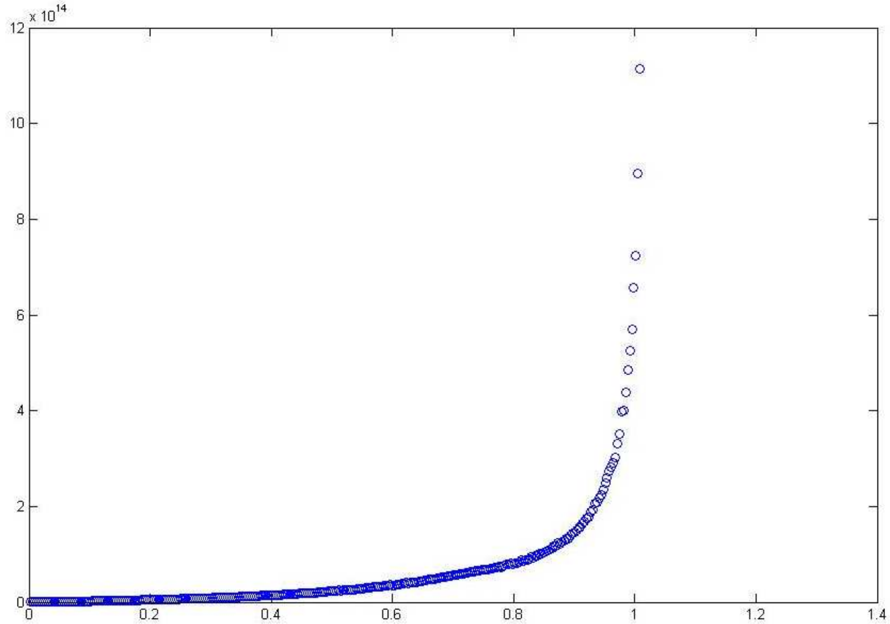

Figure 1: Collision rate versus relative density

until $c(\tau) = 3 \cdot 10^4$ collisions have been registered and for each selection of ϱ_r the collision rate has been estimated according to (2.2).

Figure 1 shows the dependence of the estimated collision rates on the relative densities ϱ_r.

The data reveal a singularity of the collision rate at $\varrho_r = 1$ (close packing) as expected.

3. A Semi-Empirical Formula for the Collision Rate

Kinematic considerations entail in the dilute range of the fluid density the formula

$$\lambda = 2rN\varrho \cdot \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} |u - v| \cdot g_\sigma(u) \cdot g_\sigma(v) du dv \tag{3.1}$$

for the collision rate in the hard disk fluid where

$$g_\sigma(v) = \frac{1}{2\pi\sigma^2} \cdot \exp\left(-\frac{1}{2\sigma^2} < v, v >\right)$$

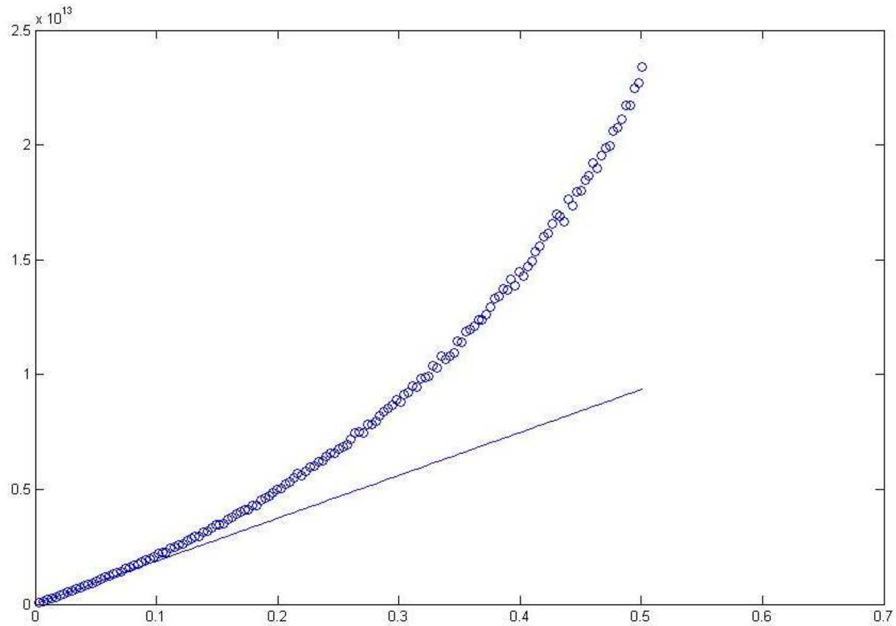

Figure 2: Theoretical and computer experimental dependence of λ on ϱ_r

denotes the density of the (Gaussian) velocity distribution and

$$\varrho = \frac{N}{V} = \frac{\varrho_r}{2\sqrt{3}r^2}$$

the particle density of the fluid.

Transforming the integral in (3.1) implies that

$$\lambda = \frac{N \cdot \varrho_r \cdot \sigma}{r} \cdot I, \tag{3.2}$$

where

$$I = \frac{1}{2\sqrt{3}\pi} \cdot \int_0^\infty \int_0^\infty \int_0^{2\pi} (r^2 + s^2 - 2rs\cos\varphi)^{1/2} \cdot rs \cdot \exp\left(-\frac{1}{2}(r^2+s^2)\right) d\varphi dr ds;$$

we have obtained for the numerical value

$$I = 1.023.$$

Figure 2 shows the comparison between prediction (3.2) of the collision rate and its computer experimental estimates for the range $0 < \varrho_r < 0.5$. Figure 2 confirms the validity of (3.2) in the dilute state of the hard disk fluid and suggests that corrections are required to predict λ in situations where the fluid is dense.

Let us consider the correction ansatz

$$\lambda = \frac{N\sigma I}{r} \cdot \varrho_r \cdot \left(1 + \beta \cdot \left(\frac{\varrho_r}{1 - \varrho_r}\right)^{\alpha}\right), \tag{3.3}$$

where parameters α and β can be estimated from computer experimental data; the least-squares estimates are

$$\widehat{\alpha} = 0.8719 \qquad \text{and} \qquad \widehat{\beta} = 1.2945.$$

(3.3) can be viewed as an extrapolation of (3.2); note that (3.3) entails a singularity of the collision rate at $\varrho_r = 1$ which complies with computer experimental results shown in Figure 1.

The average relative error in the prediction (3.3) attains 8.7%. The fact that the average relative error is significantly lower (4.4%) in the range $[0, 0.6]$ of relative density, indicates a phase transition in the range $[0.6, 1]$, which is in good agreement with [1], [2] and [4].

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