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ON THE PROPAGATION OF ULTRASONIC WAVES THROUGH THE HARD DISK FLUID

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Abstract: A local compression of the hard disk fluid is interpreted as an ultrasonic wave. The application of the kernel method from Nonparametric Statistics enables us to observe and to quantitatively evaluate the propagation of the wave in a molecular-acoustic simulation experiment. The sound velocity can be estimated by an application of the regression method to computer experimental data. A correction of a formula for the sound velocity known from Fluid Mechanics is proposed. We also report on a molecular-kinetic computer experiment in which the reflexion of a sound wave is observed.

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Key Words: kernel density estimator, molecular acoustics, linear regression

1. Introduction

An important and conceptually simple microscopic model of 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 constituting the substance are subject to thermal motion and interact through collisions.

The attractiveness of Boltzmann system has been rediscovered in the computer era when it has been recognized that Newtonian dynamics to be imposed

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on the system can be efficiently implemented in imperative programming languages. This possibility has entailed computer based studies attempting quantitatively interpretable reproduction of physical phenomena in computer experiments.

A basic physical phenomenon is connected with the zeroth law of thermodynamics; in [12] the validity of zeroth law and of Maxwell hypothesis are confirmed for hard disks based on statistical evaluation of a computer experiment. In [8] an equation of state for the hard disk fluid based on Moeschlin pressure estimator is proposed where also the thermodynamic postulate of entropy invariance under adiabatic compression is confirmed which emphasizes the thermodynamic behavior of the hard disk fluid. In [5] the phenomenon of self-diffusion is studied quantitatively entailing a realistic formula for the coefficient of self-diffusion. In [1], [6], [11] and [15] the fluid-solid phase transition is addressed for the Boltzmann system. In [7] and [10] the phenomenon of viscous fluid flow is quantitatively studied entailing a formula for the viscosity of the hard disk fluid. In [9] the computer experimental reproduction of the heat conduction through the hard sphere fluid entails a realistic formula for the thermal conductivity of noble gases and of liquid water.

In the present contribution we consider an ultrasonic wave which is realized as a local compression of the hard disk fluid and observe the propagation of the wave. The application of statistical methods to computer experimental data enables us to estimate the sound velocity. It turns out that a formula for the dependence of sound velocity on temperature of the fluid known from Fluid Mechanics has to be modified. We also realize a reflexion of the sound wave in a molecular-acoustic computer experiment.

2. Microscopic Initialization of an Ultrasonic Wave

Let us consider a 2-dimensional container

$$C := [0, L] \times [-b, b] \subset \mathbb{R}^2$$

of length $L > 0$ and width $2b > 0$. We generate initial positions of disks of radius $r > 0$ and mass $m > 0$ according to the probability distribution with Lebesgue density $f : C \to \mathbb{R}_+$ given by:

$$f(x_1, x_2) := \begin{cases} \frac{1+A\sin\left(\frac{\pi\alpha x_1}{L}\right)}{2bL(1+\frac{2A}{\pi\alpha})} & \text{if} \quad 0 \le x_1 \le L/\alpha \\ \frac{1}{2bL(1+\frac{2A}{\pi\alpha})} & \text{elsewhere.} \end{cases} \tag{2.1}$$

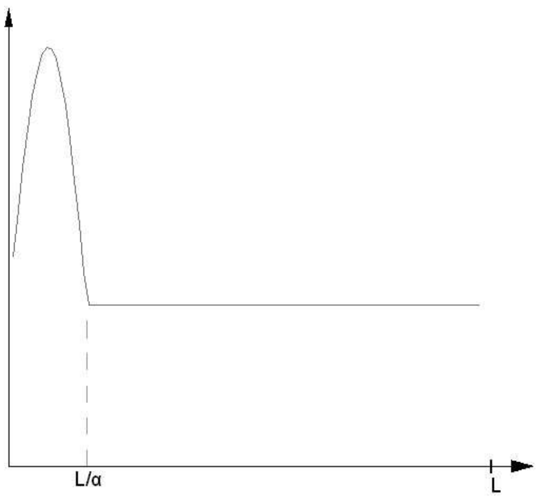

Figure 1: Density of the distribution of initial disk positions

This means that second component x_2 of a disk position vector $(x_1, x_2) \in C$ is a realization of the uniform distribution on $[-b, b]$ and the Lebesgue density of first component x_1 is locally non-uniform (cf. Figure 1) where $\alpha = 6$ and $A = 1.6$.
The generation of the initial position vectors is performed by the reject-accept method.

If we inject N non-overlapping hard disks whose positions are generated according to probability density f, then position dependent particle density ϱ_0 is approximatively given by

$$\varrho_0 \approx N \cdot f.$$

provided that the fluid consisting of the disks is not too dense. The local compression of the hard disk fluid in the proximity of the left boundary of container C can be interpreted as a sound wave.

To ensure the propagation of the wave, we generate the initial velocities of the disks inside the wave according to the 2-dimensional normal distribution

$$N(\sigma, \sigma^2) \otimes N(0, \sigma^2)$$

with the thermodynamic interpretation of variance σ^2,

$$\sigma^2 = \frac{k_B \cdot T}{m}$$

where k_B and T denotes Boltzmann constant and the temperature of the fluid, respectively. The initial velocities outside the wave are generated according to the centered normal distribution

$$N(0, \sigma^2) \otimes N(0, \sigma^2).$$

The generation of the initial velocity vectors is performed by the Box-Müller method.

3. Statistical Localization of the Ultrasonic Wave

In Section 2 the generation of the initial micro-state of the hard disk fluid confined to container C is described. Now we impose the Newtonian dynamics on the micro-constituents. The algorithm for an efficient implementation of the dynamics is presented in [12]. We are able to compute numerically the micro-state

$$(x^{(1)}(t), \ldots, x^{(N)}(t); v^{(1)}(t), \ldots, v^{(N)}(t)) \in C^N \times \mathbb{R}^{2N}$$

of the fluid at any time point $t \geq 0$ where $x^{(j)}(t) \in C$ and $v^{(j)}(t) \in \mathbb{R}^2$ denotes the position and the velocity vector of the j-th disk at time point t, respectively.

To localize the position of the fluid compression, we apply the method of kernel density estimation. For an introduction to this method cf. [3], [4], [13], [14] and [16].

Let $K : \mathbb{R} \to \mathbb{R}_+$,

$$K(x) = \frac{1}{\sqrt{2\pi}} \cdot \exp\left(-\frac{1}{2}x^2\right),$$

be the Gaussian kernel. Under the assumption that particle density ϱ_t of the fluid at time point $t \geq 0$ is independent of the vertical position coordinate, an estimate of ϱ_t is given by

$$\widehat{\varrho}_t(x_1, x_2) = \frac{1}{2bh} \cdot \sum_{j=1}^{N} K\left(\frac{x_1 - x_1^{(j)}(t)}{h}\right)$$

where $h > 0$ is an appropriate bandwidth and variable x_1 corresponds to the horizontal position coordinate. Figure 2 shows a typical estimate of ϱ_t as function of x_1.

Figure 2: Typical estimate of fluid density

A natural estimate $\widehat{X}(t)$ of the location of the sound wave at time point $t \geq 0$ is given by

$$\widehat{X}(t) := \arg \max_{x_1 \in [0,L]} \widehat{\varrho}_t(x_1);$$

$\widehat{X}(t)$ corresponds to the location of the maximal compression of the fluid at time point t as exactly as it can be estimated from the micro-data. According to our experience, the proposed kernel method outperforms the histogram estimation of particle density in the context of localization of the ultrasonic wave.

4. The Velocity of Sound

A simple formula for sound velocity $\overline{v}$ is derived in Fluid Mechanics (cf. [2], p. 44); applying this formula to the ideal gas consisting of micro-constituents of mass m yields

$$\overline{v} = \left(\frac{k_B \cdot T}{m} \right)^{1/2} \tag{4.1}$$

where T denotes temperature.

According to Section 2 we are able to initialize an ultrasonic wave in the hard disk fluid; according to Section 3 we can observe the propagation of the wave where its location can be estimated at appropriate time points. Figure 3 shows the container filled with the hard disk fluid. In the diagram above the container the horizontal axis corresponds to the position of the wave within container C and the vertical axis corresponds to experimental time. The graph shows an estimated trajectory of a wave determined by the application of estimator $\widehat{X}(t)$ introduced in Section 3 at appropriate time points. The statistical evaluation of a trajectory by linear regression yields an estimate of the sound velocity.

In a long term experiment the estimation of wave trajectories has been repeated where temperature has been varied and relative density of the fluid has been fixed: $\varrho_r = 0.002$. In Figure 4 the horizontal axis corresponds to tempera-

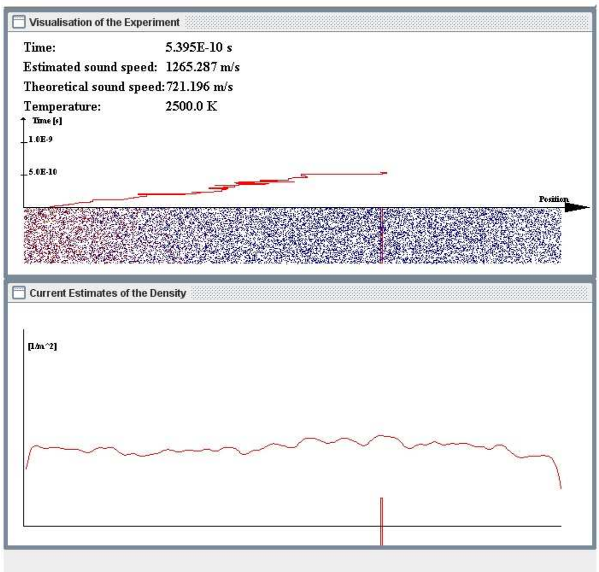

Figure 3: Propagation of the wave

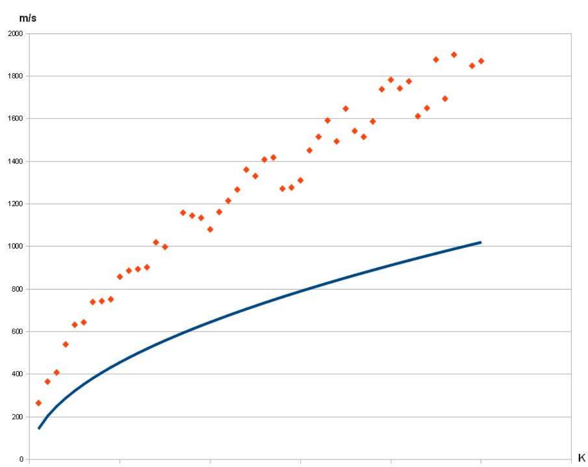

Figure 4: Sound velocity versus temperature

ture and the vertical one to sound velocity. The continuous line corresponds to prediction (4.1) and the dots correspond to sound velocity estimates obtained in the long term computer experiment. From the dots we obtain the following correction of (4.1) by the least squares method:

$$\overline{v} = 1.82 \cdot \left(\frac{k_B \cdot T}{m}\right)^{1/2} \tag{4.2}$$

Formula (4.2) is valid for the dilute state of the fluid; an extrapolation of (4.2) to dense states can be performed by the application of the state equation obtained in [8] to a statistical evaluation of an appropriate long term computer experiment.

5. Reflexion of Virtual Waves

An interesting question is, whether the phenomenon of reflexion of an acoustic wave can be reproduced in a molecular-kinetic computer experiment.

We again initialize the virtual wave according to Section 2 and let it propagate according to Section 3. Figure 5 shows container C filled with the hard disk fluid at temperature $T = 2500$ K and relative density $\varrho_r = 0.002$. In the diagram above the container the horizontal axis corresponds to the position of the wave and the vertical axis to the experimental time. An estimated trajectory of an ultrasonic wave is shown whose position has been estimated by estimator $\widehat{X}(t)$ introduced in Section 3. The trajectory shows that the virtual wave is reflected at the right boundary of container C; it shows, moreover, that the reflexion of an acoustic wave is not an instantaneous event and suggests that its duration is interrelated with the wavelength.

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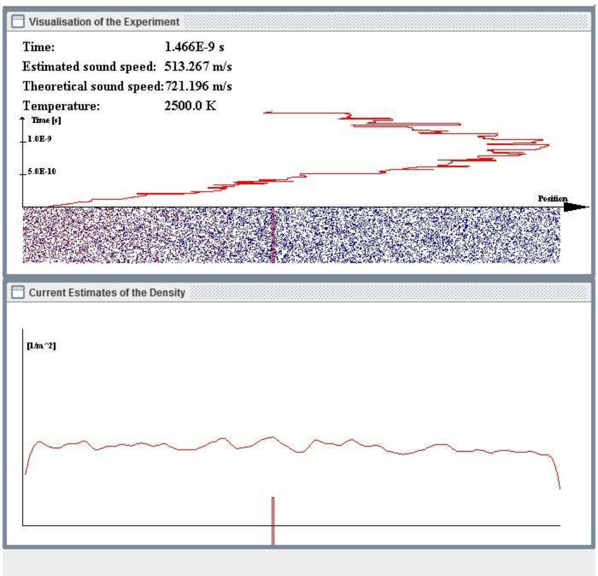

Figure 5: Reflexion of a sound wave

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