

# Kinetic approach to the Gaussian thermostat in a dilute sheared gas in the thermodynamic limit

R. van Zon\*

*Institute for Theoretical Physics, University of Utrecht, Princetonplein 5, 3584 CC Utrecht, The Netherlands*

(Received 4 May 1999)

A dilute gas of particles with short range interactions is considered in a shearing stationary state. A Gaussian thermostat keeps the total kinetic energy constant. For infinitely many particles it is shown that the thermostat becomes a friction force with constant friction coefficient. For finite number of particles  $N$ , the fluctuations around this constant are of order  $1/\sqrt{N}$ , and distributed approximately Gaussian with deviations for large fluctuations. These deviations prohibit a derivation of fluctuation-dissipation relations far from equilibrium, based on the fluctuation theorem. [S1063-651X(99)12610-2]

PACS number(s): 05.20.Dd, 05.40.-a, 05.45.-a

The interest in the relation between nonequilibrium statistical mechanics and microscopic equations of motion, which already occupied Boltzmann, has revived in recent years, on the one hand due to the development of chaos theory, but even more due to results from nonequilibrium molecular dynamics [1,2]. The main focus in the field is on stationary states. A stationary state, if it is not the equilibrium state, is the result of an external driving force. But this force performs work on the system, so it heats up (viscous heating, Ohmic heating). In simulations this is often remedied by the introduction of a mechanical thermostat: one adds a friction force,  $-\alpha \vec{v}_i$ , in the equation of motion for the velocity  $\vec{v}_i$  of each particle  $i$ , to keep the energy constant. For the thermostat variable  $\alpha$  there are several choices. One could take it constant, but then one only gets a constant energy on average. It is also possible to have  $\alpha$  time dependent, such that the total kinetic energy is constant (isokinetic Gaussian thermostat) or the total energy is constant (isoenergetic Gaussian thermostat) [2]. Neither of these thermostats are very realistic, as the dissipation of the heating would more likely occur at the boundary, where the system is in contact with a heat bath, say. Other boundary formulations where the driving force and the thermostat are combined have also been studied [3,4]. One hopes the choice of the thermostat doesn't matter in the thermodynamic limit. The equivalence of a constant  $\alpha$  thermostat, the isokinetic thermostat and isoenergetic thermostat was proposed by Gallavotti [5].

The extra term in the equations of motion destroys the Liouvillian character of the flow: a given volume in phase space will not retain that volume. As the available phase space is usually finite, this means that on average over time the volume either stays constant (conservative case) or contracts (dissipative case). In a dissipative system a stationary state can exist only on a coarse grained scale; the dissipation continues forever but on ever finer scales. This dissipation happens at a rate called the phase space contraction rate which is proportional to the average of the thermostat variable  $\alpha$ . This rate can be identified [6,7] with the irreversible entropy production [8]. If we make this identification with a physical quantity, the precise implementation (isokinetic,

isoenergetic, constant  $\alpha$ , etc.) of the thermostat should not influence the average of  $\alpha$  in the thermodynamic limit. Cohen [9] suggested that a mechanical and a physical thermostat may give the same results as long as the rate of heating is much less than the rate at which heat can be transported to the wall and absorbed there. This suggests that when the rate of heating becomes too large, the thermostat does make a difference. At that point one also expects the assumption of local equilibrium underlying nonequilibrium thermodynamics to break down, and the entropy production may no longer have the form that was used to identify it with  $\alpha$ .

We want to know which thermostat to use for analytic treatment of dilute gases in nonequilibrium stationary states. As we are interested in the limit of many particles, having to use an  $\alpha$  dependent on all these particles would certainly make work more difficult. In other analytic work on nonequilibrium stationary states, one simply takes a constant  $\alpha$  [10,11]. A sketch of a proof of the equivalence of a Gaussian isokinetic thermostat, a Gaussian isoenergetic thermostat, and a Nosé-Hoover thermostat, was already given by Evans and Sarman [12]. In this paper, we will demonstrate the equivalence of an isokinetic Gaussian thermostat and a constant thermostat in the thermodynamic limit using kinetic theory on the Boltzmann level (i.e., at low densities) for a sheared system of short range interacting particles.

## I. SHEARED GAS WITH SLLOD

We consider a dilute gas of  $N$  particles in  $d$  dimensions, under shear: the gas is contained between two plates a distance  $2L$  apart (Fig. 1). The two plates are moving in opposite directions with a velocity  $\gamma L$ . For not too large  $\gamma$  one

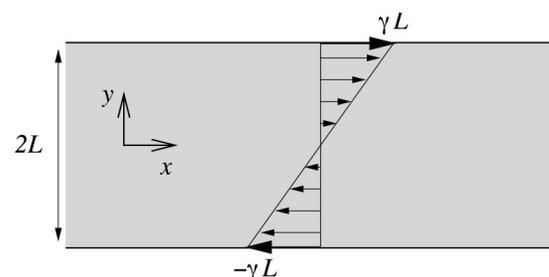


FIG. 1. Velocity profile in a gas under shear.

\*Electronic address: R.vanZon@phys.uu.nl

expects that a linear velocity profile will develop, so that the fluid velocity at  $y$  is  $\gamma y \hat{x}$ .

We are interested in bulk properties, so we let  $L$  go to infinity, while the shear rate  $\gamma$  and the density  $\rho$  are fixed. To show the equivalence of the constant  $\alpha$  thermostat and the Gaussian thermostat, it would in principle suffice just to take the horizontal dimensions infinite, but this way we can also move the boundary conditions to infinity. In the real physical system, as  $L$  get larger, the laminar flow becomes unstable and the system eventually develops turbulence. However, the thermostats we will consider assume the stability of the laminar flow [2], and suppress turbulence.

There is a well known and often used set of equations for molecular simulations that describe shear, the Sllod (so-named because of its close relationship to the Dolls tensor algorithm) equations [2]:

$$\dot{\vec{q}}_i = \vec{p}_i + \gamma y_i \hat{x}, \quad (1)$$

$$\dot{\vec{p}}_i = \vec{F}_i - \gamma p_{iy} \hat{x} - \alpha \vec{p}_i, \quad (2)$$

in which  $\vec{q}_i, \vec{p}_i$  are the phase space coordinates of particle  $i$ ,  $\alpha$  is the thermostat variable, and  $\vec{F}_i$  represents the forces between the particles. The mass of the particles is taken to be one. The shear rate is constant, but  $\alpha$  is not. It is constructed such that the kinetic energy  $K = \sum_i \|\vec{p}_i\|^2 / 2$  in the system is exactly constant, which gives

$$\alpha = \frac{1}{2K} \sum_{i=1}^N (\vec{F}_i \cdot \vec{p}_i - \gamma p_{ix} p_{iy}).$$

This is the isokinetic Gaussian thermostat. Note that  $\alpha$  depends on the positions and momenta of all the particles.

The interpretation of Eq. (1) is that  $\vec{p}_i$  is the peculiar velocity of particle  $i$  with respect to the local fluid element that has velocity  $\gamma y \hat{x}$ . In the laboratory frame, a reasonable set of equations to write down is

$$\dot{\vec{q}}_i = \vec{v}_i, \quad \dot{\vec{v}}_i = \vec{F}_i - \alpha (\vec{v}_i - \gamma y_i \hat{x}).$$

This particular form of the thermostat term is chosen because a linear velocity profile is expected, and we want the temperature to be constant, so the kinetic energy in the frame that moves with that local velocity is to be dissipated. A Boltzmann equation for the one-particle distribution function will give an appropriate description at low densities. This equation has to be supplemented by the boundary condition that the average velocities at the boundaries  $y = \pm L$  are  $\pm \gamma L$ . To get rid of the  $L$  dependence, one can transform the velocities to peculiar velocities:  $\vec{p}_i = \vec{v}_i - \gamma y_i \hat{x}$ . The average (peculiar) velocity now has to be zero at the boundaries, so when  $L \rightarrow \infty$  they have to be zero at infinity: this is the same boundary condition as for the standard Boltzmann equation. The transformation to peculiar velocities yields the Sllod equations

$$\dot{\vec{q}}_i = \vec{v}_i = \vec{p}_i + \gamma y_i \hat{x},$$

$$\dot{\vec{p}}_i = \dot{\vec{v}}_i - \gamma \dot{y}_i \hat{x} = \vec{F}_i - \alpha \vec{p}_i - \gamma p_{iy} \hat{x}.$$

## II. KINETIC APPROACH

### A. Effective motion of the thermostat

The Gaussian thermostat involves an  $\alpha$  that depends on the position and velocity of every particle, and so it varies in time. We will now derive equations of motion for the thermostat for which we do not need to know all these positions and velocities, by introducing one extra thermostat variable  $\beta$ . The derivation is in two steps: first we consider free flight, and then we take into account the effect of collisions.

During free flight  $\vec{F}$  is zero so the thermostat is given by

$$\alpha = \frac{1}{N} \sum_{i=1}^N \frac{-\gamma p_{iy} p_{ix}}{2K/N}. \quad (3)$$

Using the equations of motion, one finds that the time derivative is

$$\dot{\alpha} = -2\alpha^2 + \frac{\gamma^2}{2K} \sum_{i=1}^N p_{iy}^2 \equiv -2\alpha^2 + \beta, \quad (4)$$

where we have defined the last part as the second thermostat variable  $\beta$ :

$$\beta = \frac{1}{N} \sum_{i=1}^N \frac{\gamma^2 p_{iy}^2}{2K/N}. \quad (5)$$

We combine these to the thermostat vector  $\theta = (\alpha, \beta)$ . The time derivative of  $\beta$  is expressible again in terms of  $\alpha$  and  $\beta$ :

$$\dot{\beta} = -2\alpha\beta. \quad (6)$$

There is a conserved quantity

$$H = \frac{\alpha^2 - \beta}{2\beta^2}.$$

After change of variables to  $X = 1/(2\beta)$  and  $P = \alpha/\beta$ , this conserved quantity takes on a Hamiltonian form  $H(X, P) = \frac{1}{2}P^2 - X$ . The equations of motion are  $\dot{X} = P$  and  $\dot{P} = 1$ . The general solution, transformed back to  $\theta$ , has the form

$$\theta(t) = \frac{1}{-2H + (t - t_0)^2} \begin{pmatrix} t - t_0 \\ 1 \end{pmatrix},$$

with  $t_0$  a constant.

So far, we only considered free flight. The duration of a free flight is very small in a system of  $N$  particles: it is of the order of  $(N\nu)^{-1}$ , where  $\nu$  is the collision frequency of a single particle. In a collision,  $\theta$  changes by an amount

$$\begin{aligned} \Delta \theta &= \frac{-\gamma}{2K} \begin{pmatrix} p'_{1x} p'_{1y} + p'_{2x} p'_{2y} - p_{1x} p_{1y} - p_{2x} p_{2y} \\ -\gamma [p'^2_{1y} + p'^2_{2y} - p^2_{1y} - p^2_{2y}] \end{pmatrix} \\ &\equiv \frac{\xi(\vec{p}_1, \vec{p}_2, \hat{n})}{N}, \end{aligned}$$

where primes denote the value of the variables after collisions and  $\hat{n}$  is the collision parameter, i.e.,  $\hat{n} = (\vec{p}'_{21})$

$-\vec{p}_{21})/\|\vec{p}'_{21}-\vec{p}_{21}\|$ . As  $K$  is of the order  $N$ ,  $\Delta\theta$  is of the order of  $N^{-1}$ .  $\theta$  itself is of the order of 1. The definition makes  $\xi$  of the order of 1. During a typical free flight time of one particle, every particle in the system has collided once on average. In each collision two particles are involved, so  $N/2$  collisions have taken place in the system during this time. Thus, during one free flight time, the thermostat got  $N/2$  changes of order  $N^{-1}$  and this adds up to an effect of order 1, because, as we will see, the average of  $\Delta\theta$  is nonzero.

We will see later that the effect of the thermostat depending on all the particles, an unphysical idea in some sense, results just in a fluctuating thermostat with well defined mean and distribution. We are interested in this distribution. It will depend on the distribution of  $\Delta\theta$ , which depends on the velocity distribution in the system, which in turn is affected by the thermostat distribution. But some general properties can already be derived without this subtle interplay.

We want to write down a Boltzmann equation for the probability distribution function  $F(\theta; t)$  of the thermostat

$$\frac{\partial F}{\partial t} + \frac{\partial}{\partial \theta} \cdot (\dot{\theta} F) = \frac{\partial F}{\partial t} \Big|_c. \quad (7)$$

Here  $\dot{\theta}$  is given by Eqs. (4) and (6). The collision integral counts the number of states that are lost and gained in collisions:

$$\begin{aligned} \frac{\partial F}{\partial t} \Big|_c &= \int d\theta^* d\vec{p}_1 d\vec{p}_2 P(\vec{p}_1, \vec{p}_2, \theta^*; t) \int d\hat{n} \\ &\text{rate of } (\vec{p}_1, \vec{p}_2, \hat{n}) \\ &\times \left\{ \delta\left(\theta - \theta^* - \frac{\xi}{N}\right) - \delta(\theta - \theta^*) \right\}, \end{aligned}$$

in which  $P$  is the joint distribution of  $\vec{p}_1$ ,  $\vec{p}_2$ , and  $\theta$ , and

$$\text{rate of } (\vec{p}_1, \vec{p}_2, \hat{n}) = \frac{N}{2} \rho B(\hat{n}, \vec{p}_{21}),$$

where  $\vec{p}_{21} = \vec{p}_2 - \vec{p}_1$ .  $B$  is the rate of collisions with  $\hat{n}$  given that the colliding particles have relative velocity  $\vec{p}_{21}$ . It can be expressed in the differential cross section  $s(\hat{n}, \vec{p}_{21})$ , which measures the number of deflected particles per unit solid angle around  $\vec{p}'_{21}$  when a beam of particles of unit density is incident on one other particle. In  $d$  dimensions,

$$B(\hat{n}, \vec{p}_{21}) = \|\vec{p}_{21}\| s(\hat{n}, \vec{p}_{21}) 2^{d-1} |\hat{n} \cdot \vec{p}_{21}|^{d-2},$$

where  $\hat{p}_{21} = \vec{p}_{21}/\|\vec{p}_{21}\|$ . The last factor is the Jacobian that arises because we integrate over  $\hat{n}$  while  $s$  is defined per unit solid angle of  $\vec{p}'_{21}$ . Strictly, we ought to take  $\vec{p}_2 - \vec{p}_1 + \gamma \hat{x}(y_2 - y_1)$  instead of  $\vec{p}_{21}$ , but in the Boltzmann approach the two particles are taken at the same position when they collide. In an Enskog-type approach this would matter.

To proceed, we need an expression for  $P$  in terms of  $F$  and the one particle distribution function  $f(\vec{p})$ , which we will take normalized to 1. For  $f$ , we can also write a Boltz-

mann equation, so we will have a system of two coupled Boltzmann equations for  $f$  and  $F$ . To derive the standard Boltzmann equation [13] for  $f$ , one uses the Stosszahlansatz that states that the two-particle distribution function  $f_2(\vec{p}_1, \vec{p}_2)$  is proportional to the product of the one particle distribution functions  $f(\vec{p}_1)f(\vec{p}_2)$ , i.e., that the two particles are uncorrelated when they collide. We want a generalization of the Stosszahlansatz for  $P$ , but setting  $P(\vec{p}_1, \vec{p}_2, \theta) = f(\vec{p}_1)f(\vec{p}_2)F(\theta)$  can't quite be right for the following reason.

The Stosszahlansatz can be generated by taking the phase space density  $\rho(\{\vec{p}_i\})$  to be  $\prod_{i=1}^N f(\vec{p}_i)$ , i.e., all the particles are uncorrelated (arguably, this is too strong a condition, but it will serve to make our point). Let

$$\theta_s(\vec{p}) = \frac{N}{2K} \begin{pmatrix} -\gamma p_y p_x \\ \gamma^2 p_x^2 \end{pmatrix},$$

such that

$$\theta = \frac{1}{N} \sum_{i=1}^N \theta_s(\vec{p}_i),$$

then the quantity

$$\begin{aligned} \Pi(\vec{p}_1, \vec{p}_2, \theta) &\equiv \int d\vec{p}_3 \dots d\vec{p}_N \rho(\{\vec{p}_i\}) \delta\left(\theta - \frac{\sum_{i=3}^N \theta_s(\vec{p}_i)}{N-2}\right) \\ &\equiv f(\vec{p}_1)f(\vec{p}_2)\Phi(\theta) \end{aligned}$$

factorizes, because the delta function doesn't involve  $\vec{p}_1$  and  $\vec{p}_2$ . One easily derives that

$$P(\vec{p}_1, \vec{p}_2, \theta) = \left\{ \frac{N}{N-2} \right\}^2 \Pi\left(\vec{p}_1, \vec{p}_2, \frac{N\theta - \theta_s(\vec{p}_1) - \theta_s(\vec{p}_2)}{N-2}\right)$$

and this does not factorize.

$P$  does however factorize to zeroth order when we expand in  $N^{-1}$ . To see this, we first expand the expression for  $P$  in terms of the factorized  $\Pi$ :

$$\begin{aligned} P(\vec{p}_1, \vec{p}_2, \theta) &= f(\vec{p}_1)f(\vec{p}_2) \left\{ \Phi(\theta) \left[ 1 + \frac{4}{N} \right] \right. \\ &\quad \left. + \frac{1}{N} [2\theta - \theta_s(\vec{p}_1) - \theta_s(\vec{p}_2)] \cdot \frac{\partial \Phi}{\partial \theta} \right\} + \mathcal{O}(N^{-2}). \end{aligned}$$

$F(\theta)$  is given by  $\int d\vec{p}_1 d\vec{p}_2 P(\vec{p}_1, \vec{p}_2, \theta)$  so integrating the above formula gives a relation between  $F$  and  $\Phi$ :

$$F(\theta) = \Phi(\theta) + \frac{1}{N} \left\{ 4\Phi(\theta) + 2[\theta - \langle \theta_s \rangle] \cdot \frac{\partial \Phi}{\partial \theta} \right\} + \mathcal{O}(N^{-2}),$$

where  $\langle \theta_s \rangle = \int d\vec{p} f(\vec{p}) \theta_s(\vec{p})$ . This relation can be inverted up to order  $N^{-1}$ ,

$$\Phi(\theta) = F(\theta) - \frac{1}{N} \left\{ 4F(\theta) + 2[\theta - \langle \theta_s \rangle] \cdot \frac{\partial F}{\partial \theta} \right\} + \mathcal{O}(N^{-2}).$$

When we put this back into the the formula for  $P$ , we get  $P$  expressed in terms of  $f$  and  $F$ ,

$$P(\vec{p}_1, \vec{p}_2, \boldsymbol{\theta}) = f(\vec{p}_1) f(\vec{p}_2) \left\{ F(\boldsymbol{\theta}) + \frac{1}{N} [2\langle \boldsymbol{\theta}_s \rangle - \boldsymbol{\theta}_s(\vec{p}_1) - \boldsymbol{\theta}_s(\vec{p}_2)] \cdot \frac{\partial F}{\partial \boldsymbol{\theta}} \right\} + \mathcal{O}(N^{-2}).$$

This will serve as our Stosszahlansatz. We insert it in the collision integral and perform the  $\boldsymbol{\theta}^*$  integration,

$$\begin{aligned} \frac{\partial F}{\partial t} \Big|_c = & - \left\{ \int d\vec{p}_1 d\vec{p}_2 d\hat{n} f(\vec{p}_1) f(\vec{p}_2) \rho B(\hat{n}, \vec{p}_{21}) \frac{\boldsymbol{\xi}}{2} \right\} \cdot \frac{\partial F}{\partial \boldsymbol{\theta}} \\ & + \frac{1}{N} \left\{ \int d\vec{p}_1 d\vec{p}_2 d\hat{n} f(\vec{p}_1) f(\vec{p}_2) \rho B(\hat{n}, \vec{p}_{21}) \frac{\boldsymbol{\xi}}{2} [\boldsymbol{\theta}_s(\vec{p}_1) \right. \\ & \left. + \boldsymbol{\theta}_s(\vec{p}_2) - 2\langle \boldsymbol{\theta}_s \rangle] \right\} : \frac{\partial^2 F}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}}, \end{aligned} \quad (8)$$

where we expanded in  $N^{-1}$  once more. We define the collisional averages:

$$\begin{pmatrix} a \\ b \end{pmatrix} \equiv \frac{1}{2} \int d\vec{p}_1 d\vec{p}_2 d\hat{n} f(\vec{p}_1) f(\vec{p}_2) \rho B(\hat{n}, \vec{p}_{21}) \boldsymbol{\xi}(\vec{p}_1, \vec{p}_2, \hat{n}).$$

The Boltzmann equation for the thermostat can now be written as

$$\begin{aligned} \frac{\partial F}{\partial t} + \frac{\partial}{\partial \alpha} \{ [-2\alpha^2 + \beta + a] F \} + \frac{\partial}{\partial \beta} \{ [-2\alpha\beta + b] F \} \\ = \mathcal{O}(N^{-1}). \end{aligned}$$

This is of the form of Eq. (7) in which points in the  $\boldsymbol{\theta}$  phase space follow the effective free flight dynamics

$$\dot{\boldsymbol{\theta}} = \begin{pmatrix} -2\alpha^2 + \beta + a \\ -2\alpha\beta + b \end{pmatrix}.$$

This amounts to just adding the average effect of collisions to the change of  $\boldsymbol{\theta}$ .

Some typical trajectories in  $\boldsymbol{\theta}$  phase space are plotted in Fig. 2, both with and without the effect of collisions. When  $(a, b) \neq 0$ , it is no longer possible to derive the equations of motion from a Hamiltonian: the motion is dissipative, and there exists a fixed point  $\boldsymbol{\theta}_0 = (\alpha_0, \beta_0)$ , defined by

$$-2\alpha_0^2 + \beta_0 + a = 0; \quad 2\alpha_0\beta_0 = b. \quad (9)$$

Physically, one expects the system to heat up without a thermostat, so the thermostat should act as a friction:  $\alpha_0$  is positive. To consider the stability of the fixed point, we linearize the equation of motion around it. Writing  $\boldsymbol{\theta} = \boldsymbol{\theta}_0 + \delta\boldsymbol{\theta}$ , we get

$$\delta\dot{\boldsymbol{\theta}} = - \begin{pmatrix} 4\alpha_0 & -1 \\ 2\beta_0 & 2\alpha_0 \end{pmatrix} \delta\boldsymbol{\theta}. \quad (10)$$

The eigenvalues of the matrix are  $3\alpha_0 \pm \sqrt{\alpha_0^2 - 2\beta_0}$ .  $\beta_0$  is positive, so the fixed point is stable only if  $\alpha_0 > 0$ , consistent with the physical expectation. Furthermore, from the defini-

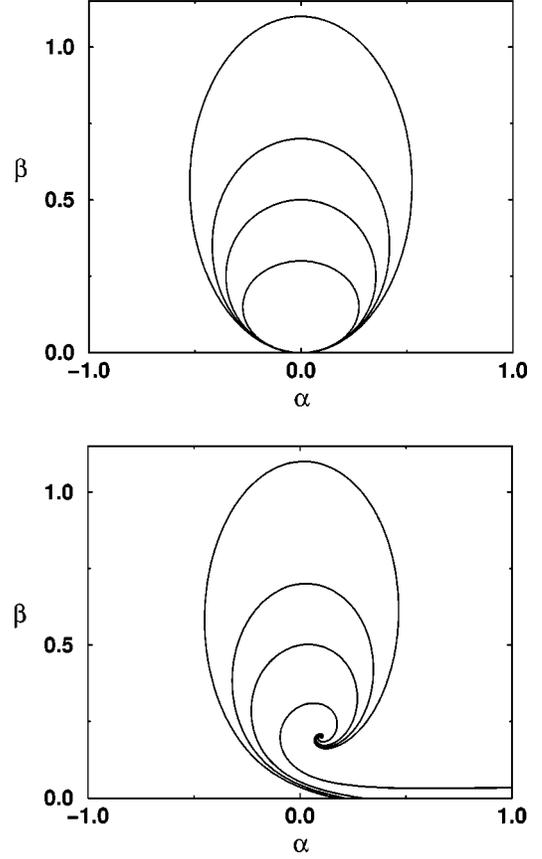


FIG. 2. Some typical  $\boldsymbol{\theta}$  trajectories of the thermostat. The first figure is without collisions, the second one is with collisional averages  $a$  and  $b$  set to the arbitrary values of  $-0.18$  and  $0.04$ , respectively.

tions in Eqs. (3) and (5), one can see that  $\alpha_0^2 < \beta_0$ , so the eigenvalues are complex and the fixed point is a stable spiral. If we take an initial distribution within the domain of attraction, all points will end up in this fixed point. Thus, in the stationary state, the distribution of the thermostat is a  $\delta$  function at  $\boldsymbol{\theta}_0$ ,

$$F(\boldsymbol{\theta}) = \delta(\boldsymbol{\theta} - \boldsymbol{\theta}_0).$$

### B. Boltzmann equation for the one particle distribution function

As we mentioned, the analysis is not complete without a second Boltzmann equation, for the one particle distribution function  $f(\vec{p}; t)$ . The difficult part *a priori* is what to do with the free flight term  $-\alpha \vec{p}_i$ . The analysis of the thermostat variables, however, showed that the  $\alpha$  is, in the stationary case, a constant, so we just replace  $\alpha$  by  $\alpha_0$ :

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial \vec{p}} \{ [-\gamma p_y \hat{x} - \alpha_0 \vec{p}] f \} = J(f, f),$$

where we considered again only the uniform case. For the stationary case we are also interested in the time derivative disappears. The collision integral is [13]

$$J(f,f)|_{\vec{p}=\vec{p}_1} = \int d\vec{p}_2 d\hat{n} \rho B(\hat{n}, \vec{p}_{21}) \{f(\vec{p}_1') f(\vec{p}_2') - f(\vec{p}_1) f(\vec{p}_2)\}.$$

In some analytic work [10,11], a constant  $\alpha$  is also used and its value is determined by demanding that the second moment  $\langle \|\vec{p}\|^2 \rangle = \int \|\vec{p}\|^2 f(\vec{p}) d\vec{p}$  is a conserved quantity. This yields

$$\alpha = -\gamma \frac{\langle p_x p_y \rangle}{\langle \|\vec{p}\|^2 \rangle}. \quad (11)$$

Note that  $\langle \|\vec{p}\|^2 \rangle$  is constant and equal to  $2K/N$ , so this choice of  $\alpha$  is very analogous to Eq. (3). In fact the solution of Eq. (9) determining the thermostat fixed point, is this  $\alpha$ , together with

$$\beta = \gamma^2 \frac{\langle p_y^2 \rangle}{\langle \|\vec{p}\|^2 \rangle}. \quad (12)$$

To show this we consider  $a$  and  $b$ ,

$$\begin{aligned} a &= \frac{-\gamma}{2K/N} \int d\vec{p}_1 d\vec{p}_2 d\hat{n} \rho B(\hat{n}, \vec{p}_{21}) f(\vec{p}_1) f(\vec{p}_2) \\ &\quad \times \frac{1}{2} \{p'_{1x} p'_{1y} + p'_{2x} p'_{2y} - p_{1x} p_{1y} - p_{2x} p_{2y}\} \\ &= \frac{-\gamma}{\langle \|\vec{p}\|^2 \rangle} \int d\vec{p}_1 d\vec{p}_2 d\hat{n} \rho B(\hat{n}, \vec{p}_{21}) p_{1x} p_{1y} \\ &\quad \times \{f(\vec{p}_1') f(\vec{p}_2) - f(\vec{p}_1) f(\vec{p}_2')\} \\ &= \frac{-\gamma}{\langle \|\vec{p}\|^2 \rangle} \int d\vec{p} J(f,f) p_x p_y, \\ b &= \frac{\gamma^2}{\langle \|\vec{p}\|^2 \rangle} \int d\vec{p} J(f,f) p_y^2. \end{aligned}$$

We insert for  $J(f,f)$  the left-hand side of the Boltzmann equation and find after partial integration

$$\begin{aligned} a &= 2\alpha_0 \frac{\langle p_x p_y \rangle}{\langle \|\vec{p}\|^2 \rangle} - \gamma^2 \frac{\langle p_y^2 \rangle}{\langle \|\vec{p}\|^2 \rangle} = 2\alpha_0 \alpha - \beta, \\ b &= 2\alpha_0 \gamma^2 \frac{\langle p_y^2 \rangle}{\langle \|\vec{p}\|^2 \rangle} = 2\alpha_0 \beta. \end{aligned}$$

Combined with Eq. (9), we see that indeed  $(\alpha_0, \beta_0) = (\alpha, \beta)$  given by Eqs. (11) and (12), is the self-consistent solution.

### III. THERMOSTAT FLUCTUATIONS

When  $N$  is finite, there are fluctuations around the thermostat value  $\alpha_0$ . One can see that the first correction, on the right-hand side of Eq. (8) has a diffusive form, with a diffusion coefficient of order  $N^{-1}$ . Combined with the drift to-

wards a fixed point from the left-hand side, this will make the thermostat distribution  $F$  peaked around this point, with a width of order  $N^{-1/2}$ . For large  $N$  the width is so small that the linearized equation, Eq. (10), is a good approximation for most of the distribution. For a linear fixed point, the distribution would be Gaussian. So the distribution  $F(\alpha, \beta)$  will become Gaussian for large  $N$ , except in the tails, where the linearized equation does not hold.

The Gaussian nature of the distribution also carries over to the finite time average of  $\alpha$ ,

$$\bar{\alpha} = \frac{1}{\tau} \int_0^\tau \alpha(t) dt.$$

For large times  $\tau$ , the thermostat will spend a long time in the neighborhood of the fixed point  $(\alpha_0, \beta_0)$ , so  $\bar{\alpha}$  will also be Gaussian distributed for large  $N$ , but, again, with deviations for large fluctuations. This all is in accordance with what one would expect from a central limit theorem.

Bonetto *et al.* [14] find a Gaussian distribution for  $\bar{\alpha}$ , but mention that the Gaussian was not what they expected, in fact, that it couldn't be Gaussian, because it would give a kind of generalized fluctuation-dissipation relation (see also [15]) when combined with the fluctuation theorem of Gallavotti and Cohen [16].

However, the deviations from the Gaussian nature at large fluctuations prohibit this derivation of far-from-equilibrium fluctuation-dissipation relations. The fluctuation theorem states that the probability  $\pi(p)$  of finding that  $\bar{\alpha}$  is  $p\alpha_0$ , divided by the probability that it is  $-p\alpha_0$ , satisfies for large  $\tau$ ,

$$\frac{\pi(p)}{\pi(-p)} = \exp[\tau dN \alpha_0 p].$$

The result was found for Anosov systems, but has been found in numerical simulations [17] and in Langevin equations [18] too, and seems to have a broader validity [19]. Combined with a Gaussian form of  $\pi$ , one gets a relation between the variance and the mean of the distribution, i.e., a kind of fluctuation-dissipation relation. The variance can be linked to a correlation function and (generalized) Green-Kubo formulas emerge [14]. But for these to hold, the Gaussian character has to be guaranteed for negative  $\bar{\alpha}$  also, and the central limit theorem, nor an extension of the analysis given here, could justify that. Recently this was acknowledged by Searles and Evans [20] and the Green-Kubo relations far from equilibrium were refuted in their molecular dynamics simulations. This does not totally explain the results of Bonetto *et al.* [14], who get a Gaussian  $\pi(p)$  for just 10 particles, the Gaussian clearly covering negative  $p$  as well. There are of course uninvestigated prefactors in the widths of the Gaussian and in range of validity.

Only when we are near equilibrium the fluctuation theorem and the central limit theorem can be combined, provided we first take the limit of the external field going to zero before we take the thermodynamic limit, even though we can take a large number of particles throughout. In such a scheme, the distribution  $\pi(p)$  is centered almost around zero, such that it always applies to some negative  $p$ .

#### IV. CONCLUSIONS

We have treated the Gaussian thermostat in a sheared system of short range interacting particles at low density using kinetic equations. We found that in the thermodynamic limit, the thermostat force becomes a friction force with a constant friction coefficient. The value of this constant was shown to be consistent with the requirement that the second moment of the one particle distribution function is conserved. This conclusion did not depend on a smallness of the shear rate, so it applies also far from equilibrium. The constant friction force has been used in other work [10,11] and the results from those should apply equally to Gaussian thermostatted systems, in the thermodynamic limit.

We briefly discussed finite  $N$  corrections. These give rise to fluctuations of the friction coefficient around its mean, of the order of  $1/\sqrt{N}$ . The fluctuations are close to Gaussian for large  $N$ , except for very large fluctuations away from the mean. Far-from-equilibrium Green-Kubo relations rely in

one derivation at least [14] on the fluctuation theorem [16], which concerns large fluctuations. The breakdown of such Green-Kubo relations recently found by Searles and Evans [20] has its origin in the deviations from the Gaussian nature for large fluctuations. Near equilibrium one doesn't need the large fluctuations.

#### ACKNOWLEDGMENTS

The author thanks Professor H. van Beijeren, Professor J.R. Dorfman, and Professor E.G.D. Cohen for valuable discussions. He acknowledges the hospitality and support of the Institute of Science and Technology at the University of Maryland in College Park and of the Rockefeller University in New York. The work reported here was supported by FOM, SMC, and by the NWO Priority Program Non-Linear Systems, which are financially supported by the "Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO)."

- 
- [1] *Proceedings of the Euroconference on the Microscopic Approach to Complexity in Non-Equilibrium Molecular Simulations. CECAM at ENS-Lyon, France, July 1996*, edited by M. Mareschal, special issue of *Physica A* **240** (1997).
- [2] D. J. Evans and G. P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids* (Academic Press, London, 1990).
- [3] N.I. Chernov and J.L. Lebowitz, *Phys. Rev. Lett.* **75**, 2831 (1995).
- [4] Ch. Dellago and H. A. Posch, *J. Stat. Phys.* **88**, 825 (1997).
- [5] G. Gallavotti, *Chaos* **8**(2), 384 (1998).
- [6] D. Ruelle, *J. Stat. Phys.* **85**, 1 (1996).
- [7] E. G. D. Cohen, *Physica A* **240**, 43 (1997).
- [8] S. R. de Groot and P. Mazur, *Non-Equilibrium Thermodynamics* (Dover Publications, New York, 1984).
- [9] E. G. D. Cohen, *Physica A* **213**, 293 (1995).
- [10] M. Lee and J. W. Dufty, *Phys. Rev. E* **56**, 1733 (1997).
- [11] J. F. Lutsko, *Phys. Rev. Lett.* **78**, 243 (1997).
- [12] D. J. Evans and S. Sarman, *Phys. Rev. E* **48**, 65 (1993).
- [13] C. Cercignani, *Theory and Application of the Boltzmann Equation* (Scottish Academic Press, Edinburgh, 1975).
- [14] F. Bonetto, G. Gallavotti, and P. L. Garrido, *Physica D* **105**, 226 (1997).
- [15] D. J. Evans and D. J. Searles, *Phys. Rev. E* **52**, 5839 (1995).
- [16] G. Gallavotti and E. G. D. Cohen, *J. Stat. Phys.* **80**, 931 (1995).
- [17] D. J. Evans, E. G. D. Cohen, and G. P. Morriss, *Phys. Rev. Lett.* **71**, 2401 (1993).
- [18] J. Kurchan, *J. Phys. A* **31**, 3719 (1998).
- [19] G. E. Crooks, *The Gallavotti-Cohen Fluctuation Theorem and the Nonequilibrium Work Relation for Free Energy Differences*, <http://xxx.lanl.gov> e-print archive, e-print cond-mat/9901352.
- [20] D. J. Searles and D. J. Evans, *The Fluctuation Theorem and Green-Kubo Relations*, <http://xxx.lanl.gov> e-print archive, e-print cond-mat/9902021.