Free cooling of particles with rotational degrees of freedom

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Abstract. Free cooling of granular materials is analyzed on the basis of a pseudo-Liouville operator. Exchange of translational and rotational energy requires surface roughness for spherical grains, but occurs for non-spherical grains, like needles, even if they are perfectly smooth. Based on the assumption of a homogeneous cooling state, we derive an approximate analytical theory. It predicts that cooling of both rough spheres and smooth needles proceeds in two stages: An exponentially fast decay to a state with stationary ratio of translational and rotational energy and a subsequent algebraic decay of the total energy. These results are confirmed by simulations for large systems of moderate density. For higher densities, we observe deviations from the homogeneous state as well as large-scale structures in the velocity field. We study non-Gaussian distributions of the momenta perturbatively and observe a breakdown of the expansion for particular values of surface roughness and normal restitution.

1 Introduction

The hard-sphere model has been a very useful reference system for our understanding of classical liquids [1]. As far as static correlations are concerned, an analytical expression for the pair correlation is available [2] and provides a good first approximation for particles interacting via smooth-potential functions. The hard-sphere model is even more important for the dynamics, because it allows for approximate analytical solutions, based on the Boltzmann equation and its generalization by Enskog to account for a finite particle diameter and pair correlations at contact [3]. The model has the additional advantage that it is particularly well suited for numerical simulations [4] and in fact many of the important phenomena of dense liquids have been observed first in simulations of hard spheres. Examples are the discovery of long-time tails [5] and two-dimensional solids [6].

Not surprisingly the model has become very popular also in the context of granular media, which are characterized by inelastic collisions of their constituents. Focusing on the rapid-flow regime, where kinetic theory should apply, generalized Boltzmann- and Enskog equations have been formulated and solved approximately [7,8,9,10,11]. The success of the Boltzmann-Enskog equation in classical fluids is based on the linearisation of the collision operator around local equilibrium. The resulting linear hermitean operator can
then be treated by standard methods of functional analysis \cite{12,13,14}. For inelastic systems no analog of the local equilibrium distribution is known. In many studies, including the present one, a homogeneity assumption is made, which is known to be unstable for dense and large enough system and long times \cite{15}. Hence the analysis is restricted to small and intermediate densities. Alternatively, one may restrict oneself to almost elastic collisions and expand around the elastic case.

Kinetic theory of rough, inelastic, circular disks was first discussed by Jenkins and Richman \cite{8}. These authors introduced two temperatures, one for the translational and one for the rotational degrees of freedom, and studied deviations from a two-temperature Maxwellian distribution, using Grad’s moment expansion. Subsequently Lun and Savage \cite{9,10} extended the approach to rough, inelastic spheres. A set of conservation equations and constitutive relations was derived from the Boltzmann equation, assuming small inelasticity and surface roughness. Goldshtein and Shapiro \cite{11} discuss in detail the homogeneous cooling state of rough spheres. They determine the asymptotic ratio of rotational to translational energy as a function of surface roughness and coefficient of normal restitution. Hydrodynamic equations and constitutive relations are derived with help of the Enskog expansion. More recently, event-driven simulations of rough spheres have been performed by McNamara and Luding \cite{16}. They investigate free cooling as a function of arbitrary surface roughness and normal restitution and compare their results to an approximate kinetic theory \cite{17,18}.

Most analytical and numerical studies of kinetic phenomena have concentrated on spherical objects so far \cite{1}. The question then arises, which of the results are specific to spherical objects and which are generic for inelastically colliding particles. A single collision of two arbitrarily shaped, but convex objects is quite difficult to describe analytically \cite{21}, set aside the problem of an ensemble of colliding grains. In this paper we have chosen the simplest non-spherical objects, needles, which allow for an analytical, albeit approximate solution and large scale simulations \cite{22}.

The paper is organized as follows. In Sec.2 we introduce the time evolution operator. For pedagogical reasons we first discuss smooth potentials and recall the formalism of a pseudo-Liouville operator for elastic, hard-core collisions. Subsequently the formalism is extended to inelastic, rough spheres and needles. The homogeneous cooling state is introduced in Sec.3. We present results for both spheres and needles, assuming a Maxwellian distribution for linear and angular momenta. We show with simulations that for dense systems of needles the assumption of homogeneity breaks down. Corrections to a Gaussian approximation are discussed in Sec.4. Finally in Sec.5 we summarize results and present conclusions. Some details of the calculation are delegated to appendices.

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1 Exceptions are computer simulations of polygonal particles \cite{19} and cellular automata models \cite{20}.
2 The Liouville operator

We are interested in macroscopic properties of systems of many particles which are themselves meso- or macroscopic, i.e. behave according to the laws of classical mechanics as opposed to quantum mechanics. In addition, our systems are granular so energy is not conserved. This means that they cannot be treated with Hamiltonian mechanics. We will present here a formalism based on the Liouville operator that enables us nevertheless to derive properties of the system under consideration.

We consider two different models: The first is a system of spheres of diameter $d$ and the second is one of (infinitely) thin rods or needles of length $L$. In order to keep the discussion as transparent as possible, the formalism of the (pseudo) Liouville operator will be demonstrated for Hamiltonian systems with smooth potentials first, for hard core potentials next, and finally for granular spheres and needles. It is interesting to note that both cases, spheres and needles, are analytically tractable so that comparisons between different geometrical particle shapes are possible.

2.1 Smooth potentials

We consider a system of $N$ classical particles of mass $m$ in a volume $V$, interacting through pairwise potentials. The system is characterized by its total energy

$$ H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j} U(r_i - r_j) $$

in terms of particle momenta $p_i$ and coordinates $r_i$. The time evolution of an observable $f(\Gamma)$, which is a function of phase space variables $\Gamma := \{r_i, p_i\}$, but does not depend on time explicitly, is given in terms of the Poisson bracket by

$$ \frac{df}{dt} = \{H, f\} =: i\mathcal{L} f. $$

This defines the Liouville operator $\mathcal{L}$. The time evolution of $f$ can then formally be written in terms of $\mathcal{L}$: $f(t) = e^{i\mathcal{L}t} f(0)$.

We decompose the Liouville operator $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\text{inter}}$ into a free-streaming part $\mathcal{L}_0$ and an operator $\mathcal{L}_{\text{inter}}$, which accounts for interactions. The definition of the Poisson bracket,

$$ \{H, f\} = \sum_j \left( \frac{\partial f}{\partial r_j} \frac{\partial H}{\partial p_j} - \frac{\partial f}{\partial p_j} \frac{\partial H}{\partial r_j} \right), $$

\[\text{Eq. (3)}\]
thus yields
\[ i \mathcal{L}_0 = \sum_j \frac{p_j}{m} \frac{\partial}{\partial r_j} \quad \text{and} \quad i \mathcal{L}_{\text{inter}} = \sum_{k<j} \frac{\partial U}{\partial r_{kj}} \left( \frac{\partial}{\partial p_j} - \frac{\partial}{\partial p_k} \right) \] (4)
with \( r_{ij} = r_i - r_j \).

### 2.2 Elastic hard-core interactions

A pseudo-Liouville operator for hard-core collisions has been formulated by Ernst et al. \[23\] and has been applied by many groups \[24\] to study the dynamic evolution of a gas of hard spheres. Collisions are instantaneous and characterized by collision rules. In a collision of two particles, numbered 1 and 2, their pre-collisional velocities \( v_1 = \frac{p_1}{m} \) and \( v_2 = \frac{p_2}{m} \) are changed instantaneously to their post-collisional values \( v_1' \) and \( v_2' \) according to
\[
\begin{align*}
v_1' &= v_1 - (v_{12} \hat{r}_{12})\hat{r}_{12} \\
v_2' &= v_2 + (v_{12} \hat{r}_{12})\hat{r}_{12}.
\end{align*}
\] (5)

We have denoted the relative velocity by \( v_{12} = v_1 - v_2 \), and \( \hat{r} = r/|r| \). The free-streaming part of the Liouville operator remains unchanged, whereas the part which accounts for interactions has to be modified because the potential is no longer differentiable in the limit of hard-core interactions. As a consequence, \( \mathcal{L} \) is no longer self-adjoint as it is for systems with smooth potentials. This is why it is called a pseudo-Liouville operator for hard-core systems. For the same reason we will need two Liouville operators below, one for forward and one for backward time evolution.

In order to construct the pseudo Liouville operator, we consider the change of a dynamical variable due to a collision of just two particles. What we need is an operator \( \mathcal{T}^{(12)} \) that
- gives the change of an observable through a collision when integrated over a short time interval containing the collision time (since the hard core interaction is non-differentiable, we have to resort to integrating over the collision instead of looking at the derivatives directly),
- only acts at the time of contact,
- only acts when the particles are approaching but not when they are receding.

The second requirement can be satisfied by \( \mathcal{T}_+^{(12)} \propto \delta(|r_{12}| - d) \), the third one demands \( \mathcal{T}_+^{(12)} \propto \Theta(-\frac{d}{dt}|r_{12}|) \), where \( \Theta(\cdot) \) is the usual Heaviside step function. In order to satisfy the first point, we use an operator \( b_+^{(12)} \) which is defined by its action on an observable \( f \) according to
\[
b_+^{(12)} f(v_1, v_2) = f(v_1', v_2'), \quad (6)\]
i.e. it simply replaces all velocities according to eqs. (5). The operator $T_+^{(12)}$ should give the change induced by a collision, so that $T_+^{(12)} \propto b_+^{(12)} - 1$. We collect the three terms and make sure to include a prefactor which is chosen such that the integration of an observable over a short time interval around the collision time yields the change of the observable, as induced by the collision rules (6). The complete expression for $T_+^{(12)}$ is thus

$$i T_+^{(12)} = \left| \frac{d}{dt} |r_{12}| \right| \delta(|r_{12}| - d) \Theta\left(- \frac{d}{dt} |r_{12}|\right) (b_+^{(12)} - 1) \). \quad (7)$$

Since the probability that three or more particles touch at precisely the same instant is zero, we only need to consider two-particle collisions and find the time-evolution operator for the system of elastically colliding hard spheres:

$$f(t) = e^{i(\mathcal{L}_0 + \mathcal{L}_\pm)t} f(0) \quad \text{for } t \geq 0 \quad (8)$$

with

$$i \mathcal{L}_\pm = \sum_{i<j} i T_\pm^{(ij)} = \sum_{i<j} \left| \frac{d}{dt} |r_{ji}| \right| \delta(|r_{ji}| - d) \Theta \left( \pm \frac{d}{dt} |r_{ji}| \right) (b_\pm^{(ij)} - 1) \). \quad (9)$$

The negative time evolution is given by $\mathcal{L}_-$, and $b^{(ij)}_-$ is the operator that replaces post-collisional velocities by pre-collisional ones.

**Extension to rough spheres** Hard-core models of elastically colliding spheres have been extended to include rotational degrees of freedom and surface roughness [8,14]. Rotational degrees of freedom offer the possibility to describe molecules with internal degrees of freedom and surface roughness is needed to transfer energy from the translational degrees of freedom to the rotational ones.

We only discuss the simplest case of identical spheres of mass $m$, moment of inertia $I$ and diameter $d$. Translational motion is characterized by the center-of-mass velocities $v_i$ and rotational motion by the angular velocities $\omega_i$. Let the surface normal $\hat{r}_{12}$ at the point of contact point from sphere 2 to sphere 1. The important quantity to model the collision is the relative velocity of the point of contact:

$$V = (v_1 - \frac{d}{2} \omega_1 \times \hat{r}_{12}) - (v_2 + \frac{d}{2} \omega_2 \times \hat{r}_{12}). \quad (10)$$

There are two contributions, firstly the center of mass velocity of each sphere, and secondly the contributions from the rotations of each sphere. The minus sign in the first parenthesis stems from the fact that the surface normal, as it was defined, points outwards for sphere 2 and inwards for sphere 1.
Now we can specify the collision rules. Primed variables always denote quantities immediately after the collision; unprimed variables denote pre-collisional quantities:

\[
\begin{align*}
\dot{r}_{12} V' &= -\dot{r}_{12} V \\
\dot{r}_{12} \times V' &= -\epsilon_t \dot{r}_{12} \times V.
\end{align*}
\] (11)

As we are still dealing with elastic spheres, energy conservation requires \( \epsilon_t = +1 \), corresponding to perfectly rough spheres, where the tangential velocity component is completely reversed. Perfectly smooth spheres \( \epsilon_t = -1 \) are also compatible with energy conservation, but reduce to the above simple case of spheres without rotational degrees of freedom, because during collision the angular velocities remain unchanged. Later, we will also admit other values for \( \epsilon_t \).

Eqs. (11) form three linearly independent equations. In addition, total momentum is conserved,

\[
v'_1 + v'_2 = v_1 + v_2,
\] (12)

and forces during a collision can only act at the point of contact. Therefore there is no torque with respect to this point and consequently we have conserved angular momentum (also with respect to the point of contact) for both particles involved:

\[
\begin{align*}
\frac{md}{2} \dot{r}_{12} \times (v'_1 - v_1) + I (\omega'_1 - \omega_1) &= 0 \\
\frac{md}{2} \dot{r}_{12} \times (v'_2 - v_2) - I (\omega'_2 - \omega_2) &= 0.
\end{align*}
\] (13)

Altogether we have 12 independent equations for 12 unknowns, namely the four vectors \( v'_i \) and \( \omega'_i \) with three components each. Solving for these, we obtain:

\[
\begin{align*}
v'_1 &= v_1 - \eta_v r_{12} - (\eta_n - \eta_t) (\dot{r}_{12} v_{12}) \dot{r}_{12} - \eta_t \frac{d}{dq} \dot{r}_{12} \times (\omega_1 + \omega_2) \\
v'_2 &= v_2 + \eta_v r_{12} + (\eta_n - \eta_t) (\dot{r}_{12} v_{12}) \dot{r}_{12} + \eta_t \frac{d}{dq} \dot{r}_{12} \times (\omega_1 + \omega_2) \\
\omega'_1 &= \omega_1 + \frac{2}{dq} \eta_v \dot{r}_{12} \times v_{12} + \frac{\eta_t}{q} \dot{r}_{12} \times (\dot{r}_{12} \times (\omega_1 + \omega_2)) \\
\omega'_2 &= \omega_2 + \frac{2}{dq} \eta_v \dot{r}_{12} \times v_{12} + \frac{\eta_t}{q} \dot{r}_{12} \times (\dot{r}_{12} \times (\omega_1 + \omega_2)).
\end{align*}
\] (14)

The dimensionless constant \( q = 4I/(md^2) \) abbreviates a frequently appearing combination of factors. We have also introduced two parameters \( \eta_n \) and \( \eta_t \), because we anticipate the more general collision rules for the inelastic case. For elastically colliding spheres, we simply have \( \eta_n = 1 \) and \( \eta_t = q/(1 + q) \) for perfectly rough and \( \eta_t = 0 \) for perfectly smooth spheres.
The pseudo-Liouville operator for elastically colliding rough spheres is still given by eq. (9) but the operator $b_{ij}^{(ij)}$ now replaces linear and angular velocities according to eqs. (14).

**Extension to rough needles** Elastic collisions of hard needles have been discussed by Frenkel et al. [25]. It is straightforward to rephrase their results in terms of a pseudo-Liouville operator [22]. The free streaming part of the Liouville operator is derived from the kinetic energy of the Hamiltonian according to the general rules of classical dynamics. Note however, that for needles, one of the moments of inertia is zero; this implies that the angular-momentum component along the corresponding axis, which points along the orientation of the needle, is also always zero. Therefore, rotations about this axis can be ignored, and $\omega$ has only two components, both perpendicular to the orientation of the needle. The center of mass coordinate of needle $i$ will be denoted by $r_i$ and its orientation by the unit vector $u_i$. The moments of inertia perpendicular to $u_i$ are equal due to symmetry and will be denoted by $I$.

The formulation of the collision rules proceeds in close analogy to rough spheres. First we determine the conditions of contact. The unit vectors $u_1$ and $u_2$ span a plane $E_{12}$ with normal

$$u_\perp = \frac{u_1 \times u_2}{|u_1 \times u_2|}.$$  \hspace{1cm} (15)

We decompose $r_{12} = r_1 - r_2$ into a component perpendicular $r_\perp^{12} = (r_{12} \cdot u_\perp) u_\perp$ and parallel $r_\parallel^{12} = (s_{12} u_1 - s_{21} u_2)$ to $E_{12}$ (see fig. 1). The rods are in contact if $r_{12} \cdot u_\perp = 0$ and simultaneously $|s_{12}| < L/2$ and $|s_{21}| < L/2$.

**Fig. 1.** Configuration of two needles projected in the plane spanned by the unit vectors $u_1$ and $u_2$
The relative velocity of the point of contact is given by
\[ V = v_{12} + s_{12} \dot{u}_1 - s_{21} \dot{u}_2. \] (16)

It is useful to introduce a set of normalized basis vectors
\[ u_1, \quad u_1^\perp = (u_2 - (u_1 u_2)u_1) / \sqrt{1 - (u_1 u_2)^2}, \quad \text{and} \quad u_\perp \] (17)
with \( u_\perp \) defined in eq. (15). Total momentum conservation is given by (12) and conservation of angular momentum with respect to the contact point reads
\[ \omega'_1 = \omega_1 + \frac{ms_{12}}{I} u_1 \times (v'_1 - v_1) \quad \text{and} \quad \omega'_2 = \omega_2 + \frac{ms_{21}}{I} u_2 \times (v'_2 - v_2). \] (18)

Three additional equations follow from the change in the relative velocity of the contact point, which is modeled in close analogy to the case of rough spheres:
\[ V'u_\perp = -Vu_\perp, \quad V'u_1 = -e_t Vu_1, \quad \text{and} \quad V'u_2 = -e_t Vu_2. \] (19)

Again, energy conservation implies \( e_t = \pm 1 \), corresponding to either perfectly rough or perfectly smooth needles (see also eq. (12)). Solving for \( v'_1 \) and \( \omega'_1 \), we obtain after a lengthy calculation:
\[ v'_1 = v_1 + \Delta v \quad \text{and} \quad v'_2 = v_2 - \Delta v \] (20)
and \( \omega'_1, \omega'_2 \) given by eq. (18). The change in velocity \( \Delta v \) can be decomposed with respect to the basis defined above, \( \Delta v = \gamma_1 u_1 + \gamma_2 u_1^\perp + \alpha u_\perp \). The coefficient \( \alpha \) is given by
\[ \alpha = - \left( 1 + \frac{ms_{12}^2}{2I} + \frac{ms_{21}^2}{2I} \right)^{-1} Vu_\perp, \] (21)
while \( \gamma_1 \) and \( \gamma_2 \) satisfy the set of linear equations
\[ \begin{pmatrix} A & B \\ B & C \end{pmatrix} \begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix} = -\frac{1 + e_t}{2} \begin{pmatrix} Vu_1 \\ Vu_1^\perp \end{pmatrix} \] (22)
with
\[ \begin{align*}
A &= 1 + \frac{ms_{12}^2}{2I} (1 - (u_1 u_2)^2), \\
B &= -\frac{ms_{21}^2}{2I} (u_1 u_2) \sqrt{1 - (u_1 u_2)^2}, \\
C &= 1 + \frac{ms_{12}^2}{2I} + \frac{ms_{21}^2}{2I} (u_1 u_2)^2.
\end{align*} \] (23)
The Liouville operator for two needles must obey the same basic requirements as for spheres. The only changes are in the condition for a collision to take place,

\[ i \hat{T}^{(12)}_+ \propto \Theta(L/2 - |s_{12}|)\Theta(L/2 - |s_{21}|)\delta(|r^\perp_{12}| - 0^+), \tag{24} \]

and in the condition that the two particles are approaching,

\[ i \hat{T}^{(12)}_+ \propto \Theta \left( -\frac{d}{dt} |r^\perp_{12}| \right). \tag{25} \]

Collecting terms and choosing the correct prefactor gives the result

\[ i \hat{T}^{(12)}_+ = \left| \frac{d}{dt} |r^\perp_{12}| \right| \Theta \left( -\frac{d}{dt} |r^\perp_{12}| \right) \times \Theta(L/2 - |s_{12}|)\Theta(L/2 - |s_{21}|)\delta(|r^\perp_{12}| - 0^+)(b^{(12)}_+ - 1). \tag{26} \]

The operator \( b^{(12)}_+ \) replaces all velocities according to eqs. (18) and (20).

### 2.3 Inelastic collision

The collision rules for rough spheres and needles are easily generalized to inelastic collisions. This will allow us to set up a formulation of the dynamics of inelastically colliding grains in terms of a pseudo-Liouville operator.

**Rough spheres** Energy dissipation is modeled by normal and tangential restitution. The collision rules imply for the change in the relative velocity of the points of contact:

\[
\hat{r}_{12} V' = -e_n \hat{r}_{12} V \\
\hat{r}_{12} \times V' = -e_t \hat{r}_{12} \times V. \tag{27}
\]

The first of these equations describes the reduction of the normal-velocity component by a non-negative factor \( e_n \). This is the well-known normal restitution. The second equation tries to describe surface roughness and friction in that it imposes a reduction or even a reversal of the tangential velocity component. It is motivated by the picture of small “bumps” on the surface which become hooked when the surfaces are very close. For all \(-1 < e_t < +1\) dissipation is present.

The change in energy is given by

\[
\Delta E = -m \left[ \frac{1}{4} - \frac{e_n^2}{4} (\hat{r}_{12} V_{12})^2 + \frac{1}{4} - \frac{e_t^2}{4} \frac{q}{1 + q} (V_{12} - (\hat{r}_{12} \omega_{12})\hat{r}_{12} - \frac{d}{2} \hat{r}_{12} \times (\omega_1 + \omega_2))^2 \right]. \tag{28}
\]
With the parameter range $0 \leq e_n \leq 1$ and $-1 \leq e_t \leq 1$, energy is only lost and never gained in a single collision.

The conservation laws for linear and angular momenta are unchanged, so we obtain the same set of equations for the post-collisional velocities as eqs. (14), with however different parameter values

$$\eta_n = \frac{1 + e_n}{2} \quad \text{and} \quad \eta_t = \frac{q \cdot e_t + 1}{1 + q}.$$ \hspace{1cm} (29)

Later we will need the inversion of eqs. (14), i.e. for given post-collisional velocities we want to determine the pre-collisional ones. This is simply done by replacing $e_t$ by $1/e_t$ and $e_n$ by $1/e_n$ in eqs. (14). The pre-collisional velocities obtained from post-collisional ones will in the following be denoted by $v''_1, v''_2, \omega''_1$ and $\omega''_2$.

**Rough needles** For hard needles we introduce normal and tangential restitution according to:

$$V'u_\perp = -e_n V u_\perp, \quad V'u_1 = -e_t V u_1, \quad \text{and} \quad V'u_2 = -e_t V u_2.$$ \hspace{1cm} (30)

The conservation laws for linear and angular momenta are the same as for the elastic case, so that one arrives at the same set of eqs. (20), the only change affecting the parameter

$$\alpha = -\frac{1 + e_n}{2} \left(1 + \frac{m s^2_{12}}{2I} + \frac{m s^2_{21}}{2I}\right)^{-1} V u_\perp.$$ \hspace{1cm} (31)

The energy loss for needles is given by

$$\Delta E = -m \frac{1 - e_t^2}{4} \left(\frac{C(V u_1)^2 - 2B(V u_1)(V u_1^\perp) + A(V u_1^\perp)^2}{AC - B^2}\right)$$

$$\quad - m \frac{1 - e_n^2}{4} \left(1 + \frac{m s^2_{12}}{2I} + \frac{m s^2_{21}}{2I}\right)^{-1} (V u_\perp)^2.$$ \hspace{1cm} (32)

It can be checked with eqs. (23) that the first term is less than 0 if and only if $-1 \leq e_t \leq 1$. Obviously, the second term is also less than 0 if $0 \leq e_n \leq 1$. Our method of modeling granular collisions of needles is therefore consistent with the constraint that energy may not be gained in a single collision.

### 2.4 Time evolution of the distribution function

We will be interested in ensemble averages of observables $f(\Gamma)$ at a time $t$ defined by:

$$\langle f \rangle (t) = \int d\Gamma \rho(\Gamma; 0)f(\Gamma; t) = \int d\Gamma \rho(\Gamma; t)f(\Gamma).$$ \hspace{1cm} (33)
Here $\rho(\Gamma; t)$ is the $N$-particle distribution function at time $t$. The average can either be taken over the initial distribution $\rho(\Gamma; 0)$ at time 0, the observable being propagated to time $t$, or equivalently over the distribution $\rho(\Gamma; t)$ at time $t$ with the unchanged observable $f(\Gamma)$. We write eq. (34) as

$$
(f)(t) = \int d\Gamma \rho(\Gamma; 0)e^{i\mathcal{L}t}f(\Gamma) =: \int d\Gamma \left(e^{i\mathcal{T}t}\rho(\Gamma; 0)\right)f(\Gamma),
$$

(34)

to define the time-evolution operator $\mathcal{T}$ which describes the time evolution of $\rho$. To determine $\mathcal{T}$ explicitly, we take the derivative of eq. (34) at time $t = 0$ for simplicity,

$$
\partial_t(f)(t)|_{t=0} = \int d\Gamma \rho(\Gamma; 0)i\mathcal{L}f(\Gamma)
= \int d\Gamma \left(\partial_t\rho(\Gamma; t)|_{t=0}\right)f(\Gamma) = \int d\Gamma \left(i\mathcal{T}\rho(\Gamma; 0)\right)f(\Gamma).
$$

(35)

The time-evolution operator of the density due to free streaming, $\mathcal{T}_0$, is easily calculated by partial integration and we get $\mathcal{T}_0 = -\mathcal{L}_0$. To find an expression for the time-evolution operator of the density due to collisions $\mathcal{T}_{+}^{(12)}$ for spheres, we use eq. (35). Phase-space coordinates before collision are denoted by $\Gamma'$, after collision by $\Gamma' = b_{+}^{(12)}\Gamma$ so that

$$
\int d\Gamma \rho(\Gamma; 0)i\mathcal{T}_{+}^{(12)}f(\Gamma) = \int d\Gamma \rho(\Gamma; 0)\delta(|\mathbf{r}_{12}| - d)\Theta\left(-\frac{d}{dt}|\mathbf{r}_{12}|\right)\frac{d}{dt}|\mathbf{r}_{12}|f(\Gamma' - f(\Gamma))\,.
$$

(36)

In the first term on the right hand side we make a coordinate transformation to the variables after collision with Jacobian $\mathcal{J} := \frac{d\Gamma'}{d\Gamma}$. We use the inverse operator of $b_{+}^{(12)}$, namely $b_{-}^{(12)}\Gamma' = \Gamma''$. Here the coordinates before collision in terms of the coordinates after collision are denoted by $\Gamma'' = \Gamma'(\Gamma')$. We note that $\frac{d}{dt}|\mathbf{r}_{12}| = \mathbf{v}_{12}\mathbf{r}_{12}$ and rewrite the first term

$$
\int d\Gamma \rho(\Gamma; 0)\delta(|\mathbf{r}_{12}| - d)\Theta\left(-\frac{d}{dt}|\mathbf{r}_{12}|\right)\frac{d}{dt}|\mathbf{r}_{12}|f(\Gamma') = \int d\Gamma' \mathcal{J} \rho(\Gamma''; t)\delta(|\mathbf{r}_{12}| - a)\Theta(-\mathbf{v}'_{12}\mathbf{r}_{12})|\mathbf{v}'_{12}\mathbf{r}_{12}|f(\Gamma')
$$

(37)

Next we rename $\Gamma'$ by $\Gamma$ and make use of $\mathbf{v}_{nm}\mathbf{r}_{nm} = -\frac{1}{\epsilon_n}(\mathbf{v}_{nm}\mathbf{r}_{nm})$. This allows us to identify the time-evolution operator of the distribution function, $\mathcal{T}_{+}^{(12)}$, by

$$
\mathcal{T}_{+}^{(12)} = \delta(|\mathbf{r}_{12}| - d)\left|\frac{d}{dt}|\mathbf{r}_{12}|\right|\left(\Theta\left|\frac{d}{dt}|\mathbf{r}_{12}|\right|\mathcal{J} b_{+}^{(12)} - \Theta\left(-\frac{d}{dt}|\mathbf{r}_{12}|\right)\right).
$$

(38)
It is common to rewrite eq. (38) by multiplying it with \( \int d\sigma \delta(\sigma - r_{12}) \) so that we can replace \( r_{12} \) by \( \sigma \) in eq. (38). In the second term the integral transformation \( \sigma \to -\sigma \) is done and we integrate over \( |\sigma| \). We obtain in \( D \) dimensions

\[
i T_+^{(12)} = d^{D-1} \int_{v_{12} \sigma > 0} d\hat{\sigma} (v_{12} \hat{\sigma}) \left( \frac{\mathcal{J}}{\epsilon_r} \delta(r_{12} - d\hat{\sigma}) b^{(12)}_0 - \delta(r_{12} + d\hat{\sigma}) \right).
\]

(39)

Finally, we note that \( t = 0 \) is not special since we have only chosen it for the sake of simplicity. Hence we have derived the time-evolution operator for the \( N \)-particle distribution function \( \rho(\Gamma; t) \) which is given by the pseudo-Liouville equation

\[
\partial_t \rho(\Gamma; t) = i \left( -L_0(\Gamma) + \sum_{i<j} T_{+}^{(ij)} \right) \rho(\Gamma; t).
\]

(40)

A similar procedure yields the time evolution operator for the distribution of needles.

3 Homogeneous cooling state

We are interested in the time evolution of a gas of freely cooling rough spheres or needles which is dominated by two-particle collisions, as discussed in the previous section. We aim at a description in terms of macroscopic quantities and focus on the decay in time of the average kinetic energy of translation and rotation, defined as

\[
\langle E_{\text{tr}} \rangle(t) = \frac{m}{2N} \sum_i \int d\Gamma \rho(\Gamma; t) v_i^2 =: \frac{D_{\text{tr}}}{2} T_{\text{tr}}(t),
\]

\[
\langle E_{\text{rot}} \rangle(t) = \frac{I}{2N} \sum_i \int d\Gamma \rho(\Gamma; t) \omega_i^2 =: \frac{D_{\text{rot}}}{2} T_{\text{rot}}(t).
\]

(41)

Here \( D_{\text{tr}} \) and \( D_{\text{rot}} \) denote the total number of translational and rotational degrees of freedom respectively. It is impossible to compute the above expectation values exactly and we have to resort to approximations. We assume that the \( N \)-particle probability distribution \( \rho(\Gamma; t) \) is homogeneous in space and depends on time only via the average kinetic energy of translation and rotation:

\[
\rho_{\text{HCS}}(\Gamma; t)_{\text{HCS}} \sim W(r_1, \ldots, r_N) \hat{\rho}(\{v_i, \omega_i\}; T_{\text{tr}}(t), T_{\text{rot}}(t)).
\]

(42)

The function \( W(r_1, \ldots, r_N) \) gives zero weight to overlapping configurations and 1 otherwise. Needles have vanishing volume in configuration space, so
that $W \equiv 1$. We shall furthermore assume that $\hat{\rho}$ factors neglecting correlations of the velocities of different particles. In the simplest approximation we take $\hat{\rho}$ to be Gaussian in all its momentum variables

$$\hat{\rho}(\{v_i, \omega_i\}; T_{tr}(t), T_{rot}(t)) \propto \exp \left[ -N \left( \frac{E_{tr}}{T_{tr}(t)} + \frac{E_{rot}}{T_{rot}(t)} \right) \right]. \quad (43)$$

In the next section, we shall discuss non Gaussian distributions and shall compute corrections perturbatively.

To determine the time dependence of $T_{tr}(t)$ and $T_{rot}(t)$ we take time derivatives of eqs. (41) and use the identity

$$\frac{d}{dt} \langle f \rangle(t) = \int d\Gamma \langle \frac{d}{dt} \rho(\Gamma, t) \rangle f(\Gamma) = \int d\Gamma (iL \rho(\Gamma, t)) iL f(\Gamma).$$

Then $\rho(\Gamma, t)$ is replaced by $\rho_{HCS}(\Gamma; t)$, resulting in

$$\frac{d}{dt} T_{tr}(t) = \frac{2}{D_{tr}} \int d\Gamma \rho_{HCS}(\Gamma; t) i \mathcal{L} E_{tr} = \frac{2}{D_{tr}} \langle i \mathcal{L} E_{tr} \rangle_{HCS} \quad \text{and}$$

$$\frac{d}{dt} T_{rot}(t) = \frac{2}{D_{rot}} \int d\Gamma \rho_{HCS}(\Gamma; t) i \mathcal{L} E_{rot} = \frac{2}{D_{rot}} \langle i \mathcal{L} E_{rot} \rangle_{HCS}. \quad (44)$$

All that remains to be done are high dimensional phase-space integrals, the details of which are delegated to appendices A and B, for spheres and needles.

### 3.1 Results for spheres

After integration over phase space has been performed (see Appendix A for details), we find

$$\frac{D_{tr}}{2} \frac{d}{dt} T_{tr}(t) = \langle i \mathcal{L} E_{tr} \rangle_{HCS} = -G A T_{tr}^{3/2} + G B T_{tr}^{1/2} T_{rot},$$

$$\frac{D_{rot}}{2} \frac{d}{dt} T_{rot}(t) = \langle i \mathcal{L} E_{rot} \rangle_{HCS} = G B T_{rot}^{3/2} - G C T_{tr}^{1/2} T_{rot}, \quad (45)$$

with the always positive constants $A$, $B$, $C$, and $G$ depending on space dimensionality $D$. In two dimensions the constants in eqs. (43) are given by

$$G = 4d N V \sqrt{\pi \frac{1}{m}} g(d), \quad A = \frac{1 - e_n^2}{4} + \frac{\eta_x}{2} (1 - \eta_x),$$

$$B = \frac{\eta_x^2}{2q}, \quad C = \frac{\eta_x}{2q} \left( 1 - \frac{\eta_x}{q} \right). \quad (46)$$

and in three dimensions

$$G = 8d^2 N V \sqrt{\pi \frac{1}{m}} g(d), \quad A = \frac{1 - e_n^2}{4} + \eta_x (1 - \eta_x),$$

$$B = \frac{\eta_x^2}{q}, \quad C = \frac{\eta_x}{q} \left( 1 - \frac{\eta_x}{q} \right). \quad (47)$$
The pair correlation function at contact, $g(d)$, is defined in the usual way [1]. A detailed discussion of these results, and in particular the dependence of free cooling on $e_n$ and $e_t$, can be found in [18].

The Enskog value [14, 28] of the collision frequency $\omega_E$, i.e. the average number of collisions which a particle suffers per unit time in $D$ dimensions is given by

$$\omega_E := S_D \frac{N}{V} g(d) a^{D-1} \sqrt{\frac{T_{tr}(t)}{\pi m}}.$$  \hfill (48)

$S_D$ is the surface of a unit sphere in $D$ dimensions. Note that always $\omega_E \propto GT^{1/2}$. We define dimensionless time $\tau$ by $d\tau = \omega_E dt$ so that $\tau$ counts the collisions that on average each particle has suffered until time $t$. In a simulation this would simply be done by counting the number of collisions. The functional dependence of the two temperatures on $\tau$ is determined by

$$\frac{d}{d\tau} T_{tr} = -aT_{tr} + bT_{rot},$$ \hfill (49)

$$\frac{d}{d\tau} T_{rot} = bT_{tr} - cT_{rot}$$ \hfill (50)

with properly defined $a, b, c$. Eq. (49) has a simple interpretation: In a given short interval $\Delta t$ a number of $\Delta \tau$ collisions occur. Due to these collisions translational energy decreases by an amount given by the first term, but there is also a gain term, reflecting that rotational energy is transferred to translational energy. The solution of eqs. (49, 50) can be written as

$$T_{tr} = c_1 K_+ \exp(-\lambda_+ \tau) + c_2 K_- \exp(-\lambda_- \tau),$$ \hfill (51)

$$T_{rot} = c_1 \exp(-\lambda_+ \tau) + c_2 \exp(-\lambda_- \tau),$$ \hfill (52)

$$K_\pm = \frac{1}{2b} \left( c - a \pm \sqrt{(c-a)^2 + 4b^2} \right),$$ \hfill (53)

$$\lambda_\pm = \frac{1}{2} \left( c \mp \sqrt{(c-a)^2 + 4b^2} \right).$$ \hfill (54)

The constants $c_1$ and $c_2$ are determined by the initial conditions and $\lambda_- > 0$, $\lambda_+ > 0$ and $\lambda_- > \lambda_+$ holds for all $e_t, e_n$. Hence for long times the ratio of $T_{tr}/T_{rot}$ is determined by $K_+.$

We now assume that the ratio $T_{tr}/T_{rot}$ has reached its asymptotic value $K_+$ for some $\tau > \tau_0$ or equivalently $t > t_0$ and substitute $T_{rot} = T_{tr}/K_+$ into eq. (47) we obtain

$$\frac{d}{dt} T_{tr} = -FT^{3/2}.$$ \hfill (55)

The resulting equation is of the same functional form as for homogeneous cooling of smooth spheres, except for the coefficient $F$, which contains all the
dependence on system parameters. Its solution is given by

\[ T_{tr} = \frac{T_{tr}(t_0)}{\left[1 + T_{tr}(t_0)^{1/2}(F/2)(t-t_0)\right]^2} \sim \frac{1}{(Ft/2)^2}, \quad (56) \]

Haff's law of homogeneous cooling. We have determined two time scales, first an exponentially fast decay (measuring time in collisions) towards a state where we find a constant ratio of translational and rotational energy. As long as dissipation is small, we approximate the Enskog-collision frequency for sufficiently short times by its initial value \( \omega(t) \sim \omega(0) \) so that we find exponential behavior also in real time. The second stage of relaxation is characterized by a slow, algebraic decay of both energies, such that their ratio remains constant. These two time regimes are clearly seen in the numerical solution of eq. (46) for initial conditions \( T_{tr}(0) = 1 \) and \( T_{rot}(0) = 0 \), i.e. a system prepared in an equilibrium state of perfectly smooth spheres. We show in fig. 2a) in a double logarithmic plot the time dependence of the total energy

\[ E = \frac{3}{2}(T_{tr}(t) + T_{rot}(t)) \]

and the ratio \( T_{tr}(t)/T_{rot}(t) \). Time is plotted in units of \( GT_{tr}^{1/2}(0) \). We have chosen \( e_n = 0.9 \) and \( e_t = -0.8 \).

![Fig. 2.](image)

3.2 Results for needles

In the case of needles we restrict ourselves to the case of perfectly smooth needles, i.e. \( e_t = -1 \). After some lengthy algebra, presented in appendix B,
eq. (44) can be cast in the following form
\[
\frac{2 \dot{T}_{tr}}{\gamma_n T_{tr}^{3/2}(1 + e_n)} = -\int d^2 r \frac{(1 + \frac{T_{rot}}{T_{tr}} kr^2)^{1/2}}{1 + k r^2} + \frac{1 + e_n}{2} \int d^2 r \frac{(1 + \frac{T_{rot}}{T_{tr}} kr^2)^{3/2}}{(1 + k r^2)^2}, \tag{57}
\]

\[
\frac{4 \dot{T}_{rot}}{3 \gamma_n T_{tr}^{3/2}(1 + e_n)} = -\int d^2 r \frac{\frac{T_{rot}}{T_{tr}} kr^2 (1 + \frac{T_{rot}}{T_{tr}} kr^2)^{1/2}}{1 + k r^2} + \frac{1 + e_n}{2} \int d^2 r \frac{kr^2 (1 + \frac{T_{rot}}{T_{tr}} kr^2)^{3/2}}{(1 + k r^2)^2}, \tag{58}
\]

with \( \gamma_n = \frac{(2 NL^2 \sqrt{\pi})}{(3 V \sqrt{m})} \) and \( k = \frac{(mL^2)}{2 I} \). The two dimensional integration extends over a square of unit length, centered at the origin.

In fig. 2b) we plot the numerical solution of eqs. (57,58) for \( e_n = 0.8 \) and \( k = 6 \) \( (k = 6 \) corresponds to a homogeneous mass distribution along the rod) as a function of time in units of \( \gamma_n \sqrt{T_{tr}(0)} \). In addition we have performed simulations of a system of 10000 needles, confined to a box of length 24 \( L \). We show the total kinetic energy \( E = \frac{3}{2} T_{tr} + T_{rot} \) (in units of \( T_{tr}(\tau = 0) \)) and the ratio \( T_{tr}/T_{rot} \). Analytical theory and simulation are found to agree within a few percent over eight orders of magnitude in time. \( \tau \) has been chosen as initial condition). For needles we observe an even clearer separation of time scales. The decay of \( T_{tr}/T_{rot} \) to a constant value \( K_+ \) happens on a time scale of order one. In this range of times the total kinetic energy \( E \) remains approximately constant (on a logarithmic scale) and decays like \( t^{-2} \) only after translational and rotational energy have reached a constant ratio. We plug the ansatz \( K_+ T_{rot} = T_{tr} \) into eqs. (57,58) and recover Haff’s law also for needles. To determine the constant \( K_+ \) we use \( K_+ T_{rot} - T_{tr} = 0 \), which yields an implicit equation for \( c \). Equipartition holds for all values of \( e_n \) if \( k = \frac{(mL^2)}{2I} \) is set to particular value \( k^* = 4.3607 \), given as the solution of

\[
(1 - e_n^2) \int d^2 r \frac{1 - \frac{4}{3} k^* r^2}{\sqrt{1 + k^* r^2}} = 0.
\]

For \( k < k^* \) we find \( T_{tr} < T_{rot} \) and for \( k > k^* \), \( T_{tr} > T_{rot} \). Hence the distribution of mass along the rods determines the asymptotic ratio of rotational and translational energy, including equipartition as a special case.

### 3.3 Breakdown of homogeneity in dense systems of needles

It is well known that dense and large systems of inelastically colliding spheres exhibit clustering so that the assumption of homogeneity breaks down and
deviations from Haff's law of homogeneous cooling are observed. To investigate inhomogeneities for dense systems of needles we measure hydrodynamic quantities, i.e. we define local variables as the density field, the translational and rotational flow field and the local rotational and translational kinetic energy. In order to take local averages over small volumes, we divide the simulation box into cells whose sizes are small compared to the box size but large enough to give a reasonable statistics. We choose cell size, such that on average about 25 needles are in each cell. For each cell indexed by α we compute the number density \( \rho_\alpha := \frac{1}{V_{\text{cell}}} \sum_{i \in \text{cell}_\alpha} 1 = \langle 1 \rangle_\alpha \), the translational energy per particle \( \rho_\alpha E^{tr}_\alpha = \langle \frac{m}{2} v_i^2 \rangle_\alpha \) and the hydrodynamic temperature \( T^{tr}_\alpha = E^{tr}_\alpha - \frac{m U_\alpha^2}{2} \) defined by fluctuations around the flow field \( \rho_\alpha U_\alpha = \langle v \rangle_\alpha \). The corresponding observables of the rotational degrees of freedom are the rotational energy per particle \( E^{rot}_\alpha \), the hydrodynamic rotational temperature \( T^{rot}_\alpha \) and the rotational flow field \( \Omega_\alpha \).

To check for spatial clustering, we compare the statistics of fluctuations of the local density, velocity and translational energy for elastic and inelastic systems. As an example we show in fig. 3 the histogram of the deviation of the local density \( \delta \rho_\alpha = \rho_\alpha / n - 1 \). We performed simulations of a dense and large system of 20000 needles confined to a volume with linear dimension \( 12L \) and \( e_\alpha = 0.9 \). The initial distribution is uniform, corresponding to the equilibrium state of an elastic system. As the system develops in time with particles colliding inelastically, we observe that the distribution broadens, a clear indication that regions of large density have developed. Histograms of the local translational and rotational energies look very similar.

Inelastic hard spheres without surface roughness tend to move more and more parallel so that large scale structures in the velocity field develop. In such a state most of the kinetic energy is to be found in the energy of the flow field, whereas the energy of the fluctuations around the flow

\[ \text{fig. 3. Histogram of density fluctuations in the initial state and after 560 Collisions per particle. It is obvious that regions with high density have developed.} \]
field is small. A quantitative measure for this effect is the ratio of the total energy of the flow to the total internal energy of fluctuations:

\[ S_{tr} := \frac{\sum_{\alpha} \frac{m}{2} \rho_{\alpha} U_{\alpha}^2}{\sum_{\alpha} \rho_{\alpha} T_{tr,\alpha}} \] and the analogous quantity \( S_{rot} \) for the rotational degrees of freedom. In fig. 4 we show \( S_{tr} \) and \( S_{rot} \) as a function of time, measured in collisions per particle. We observe an increase of \( S_{tr} \) by a factor of 50, whereas \( S_{rot} \) increases only by about 50%. Hence the large scale structures in the flow field are much more pronounced for the translational velocity. In the fig. 5 we show the flow field after 600 collisions per particle.

\[ \text{Fig. 4. Ratio } S_{tr} \text{ and } S_{rot} \text{ of the local macroscopic energy to the local temperature for the translational (rotational) degrees of freedom as a function of the number of collisions per particle.} \]

We observe two shear bands (note the periodic boundary conditions) in which the flow field is to a large degree aligned. In periodic boundary conditions stable shear bands have to be aligned with the walls of the box.

\[ \text{Fig. 5. Flow field after 600 collisions per particle} \]
How does the organization of the flow field influence the decay of the average energy in the system? Brito and Ernst [30] have suggested a generalized Haff’s law to describe the time dependence of the kinetic energy of smooth inelastically colliding spheres even in the non-homogeneous state. They found that in the late state where one finds a well developed flow field the energy decays like $\tau^{-D/2}$ in $D$ dimensions. As in section 3.1 $\tau$ is the average number of collisions suffered by a particle within time $t$. In fig. 6 we compare the data of the simulation with the solution of eqs. (57,58) and in the inset we plot $T_{tr}$ as a function of $\tau$ and compare it to $\tau^{-3/2}$. We can not confirm a $\tau^{-3/2}$ law, but by inspection of fig. 6 we see that the range of correlations are already of the order of the system size, so that finite size effects – not taken into account in the theory of Brito and Ernst – may be dominating. To simulate larger systems and longer runs has not been possible because simulations of dense systems are rather time consuming [22].

![Fig. 6.](image)

**Fig. 6.** Data of simulations for translational and rotational temperature as a function of time (units of $\gamma_n \sqrt{T_{tr}(0)}$) are compared to the numerical solution of eq. (57,58) and to $\tau^{-3/2}$. The inset shows $T_{tr}$ as a function of $\tau$ and $\tau^{-3/2}$.

4 **Non-Gaussian Distribution**

In this section we keep the assumption of homogeneity and factorization of the $N$-particle distribution function, but go beyond the approximation of a purely Gaussian state. Initially the system is prepared in a Gaussian state, so that deviations from the Gaussian should be small for short times and perturbation theory can be used to check the range of validity of the Gaussian approximation. We expand the one particle distribution function in generalized Laguerre polynomials (for a definition see [31]) around the Gaussian with
time dependent variances. We define an average velocity \( v_0(t) = \sqrt{2T_{nr}(t)/m} \) and \( \omega_0(t) = \sqrt{2T_{rot}(t)/I} \) and scale linear velocities by \( v_0(t) \) and angular velocities by \( \omega_0(t) \). The general ansatz for the N-particle distribution function of the homogeneous cooling state then reads

\[
\rho(\Gamma, t) \sim W(r_1, ..., r_N) \prod_{i=1}^{N} \rho_i(v_i, \omega_i, t), \quad \text{and}
\]

\[
\rho_i(v_i, \omega_i, t) = \frac{1}{Z(t)} \exp \left( -\left( \frac{v_i}{v_0(t)} \right)^2 - \left( \frac{\omega_i}{\omega_0(t)} \right)^2 \right) \sum_{n,m=0}^{\infty} a_{n,m}(t) L_n^\alpha \left( \left( \frac{v_i}{v_0(t)} \right)^2 \right) L_m^\beta \left( \left( \frac{\omega_i}{\omega_0(t)} \right)^2 \right). \quad (59)
\]

We have introduced the abbreviations \( \alpha = D_{nr}/2 - 1 \) and \( \beta = D_{rot}/2 - 1 \). The average linear and angular velocities, \( v_0(t) \) and \( \omega_0(t) \), are time dependent and so are the coefficients \( a_{n,m}(t) \) of the double expansion. At time \( t = 0 \) the system is equilibrated with temperature \( T \) so that \( \frac{m}{2} v_0^2 = \frac{D_{nr}}{2} T \) and \( I \omega_0^2 = \frac{D_{rot}}{2} T \) and hence \( a_{n,m}(t) = 0 \).

The factor \( Z(t) \) follows from the proper normalization,

\[
Z(t) = v_0^{D_{nr}} \omega_0^{D_{rot}} \sqrt{\pi}^{D_n} \sqrt{\pi}^{D_{rot}} a_{0,0} ,
\]

and we require that \( v_0(t) \) and \( \omega_0(t) \) be determined by the conditions

\[
\int d\Gamma v_0^2 \rho(\Gamma, t) = \frac{D_{nr}}{2} v_0^2(t) \quad \text{and} \quad \int d\Gamma \omega_0^2 \rho(\Gamma, t) = \frac{D_{rot}}{2} \omega_0^2(t). \quad (61)
\]

The orthogonality relations of the Laguerre polynomials imply \( a_{1,0}(t) = a_{0,1}(t) = 0 \) for all times \( t \) and

\[
a_{n,m}(t) = \frac{1}{(n+\alpha)} \frac{1}{(m+\beta)} \int d\Gamma \rho(\Gamma, t) L_n^\alpha \left( \left( \frac{v_1}{v_0(t)} \right)^2 \right) L_m^\beta \left( \left( \frac{\omega_1}{\omega_0(t)} \right)^2 \right). \quad (62)
\]

The binomial coefficients are denoted by \( \binom{a}{b} \) and we choose \( a_{0,0} = 1 \).

Taking the time derivative of eqs. (51,52) one gets the full time dependence of the homogeneous cooling state given by the time dependence of all its momenta. Taking time derivatives of the right hand side of eq. (52) one has to take into account the time dependence of \( \rho(\Gamma, t) \), which is determined by \( \mathcal{E} \) as well as the time dependence of \( L_n^\alpha \left( \frac{v_1}{v_0(t)} \right)^2 L_m^\beta \left( \frac{\omega_1}{\omega_0(t)} \right)^2 \) via \( v_0(t) \) and \( \omega_0(t) \), which follows from eq. (51).

Assuming that all \( a_{n,m} \) are stationary in time and that \( v_0/\omega_0 = \mu \) is constant we get an infinitely large, nonlinear system of equations. To make further progress we truncate the expansion in eq. (53) and take into account only \( a_{n,m} \) for \( n+m \leq 2 \). We also neglect in the system of equations products
of different \( a_{n,m} \), which we assume to be of higher order. We show results for \( a_{0,2} \) in fig. 7 for fixed \( e_n = 0.9 \) as a function of \( e_t \). Deviations from the Gaussian vanish for perfectly smooth spheres and are found to increase dramatically for \( e_t \to -0.9 \). Deviations from the Gaussian distribution are also small for perfectly rough spheres which is unexpected, because rotational degrees of freedom are coupled to translational ones and \( e_n = 0.9 \). In fact deviations stay small for a broad range of values of \( e_t \gtrsim -0.75 \). We don’t consider it meaningful to plot the theoretical result, once a divergence of \( a_{0,2} \) has occurred. We measured \( a_{0,2} \) in simulations of small systems. Thereby we avoid clustering but have to bear with poor statistics. The simulations confirm the increase of \( a_{0,2} \) around \( e_t = -0.7 \) in agreement with the perturbation expansion.

Goldshtein and Shapiro [11] propose a similar set of momentum equations but they solve it only to lowest order, resulting therefore in the same asymptotic ratio \( \mu \) as given in eq. (53).

![Fig. 7. Coefficient \( a_{0,2} \) for \( e_n = 0.9 \) as a function of \( e_t \). Theory (straight line) and simulations (circles) are compared.](image)

5 Conclusion

Two simple models of granular particles with rotational degrees of freedom are discussed: Rough spheres or discs and, as an example for non-spherical particles, needles. We focus on the simplest collision rules, which allow for a transfer of translational energy to rotational degrees of freedom. For spheres this is achieved by tangential restitution (in addition to normal restitution), for needles normal restitution is sufficient. We show that the time evolution
can be formulated in terms of a pseudo Liouville operator, thereby generalizing previous work on elastic collisions to inelastic ones. The presented formalism is general enough to include more realistic collision rules, for example Coulomb friction for small angles of impact and tangential restitution for large angles. Work along those lines can be found in [32].

The computation of non-equilibrium expectation values, like e.g. the relaxation of kinetic energy, require approximations. These are formulated for the $N$-particle distribution function, which we assume to be homogeneous in space and depend on time only via the average translational and rotational energy, $T_{\text{tr}}$ and $T_{\text{rot}}$. The distribution of linear and angular momenta is expanded in Laguerre polynomials around a Gaussian state with time dependent width, $T_{\text{tr}}$ and $T_{\text{rot}}$. The zeroth order approximation, i.e. a pure Gaussian, leads to two coupled differential equations for the two temperatures. In both systems, spheres and needles, the relaxation of translational and rotational kinetic energy is characterized by two time scales: (1) An exponentially fast decay towards a state with constant ratio of translational to rotational energy and (2) an algebraically slow decay of the whole energy, such that the above ratio keeps constant in time. The theoretically predicted cooling dynamics is supported by computer simulations of systems of small or moderate density, where no shearing or cluster instability is observed and the system remains homogeneous [18,22].

To study deviations from the Gaussian state, we restrict ourselves to rough spheres and truncate the expansion in Laguerre polynomials, keeping the first three terms (the first order term for smooth spheres has already been computed in [33]). This perturbative approach is shown to break down for certain values of $\epsilon_t$ and $\epsilon_n$, where deviations from the Gaussian are shown to diverge. These results are confirmed by simulations. We indicate, how a more general expansion with time dependent coefficients can be achieved. For totally smooth spheres this expansion has been performed up to fifth order [34]. It predicts an exponentially fast decay of the coefficients to their stationary values in agreement with simulations and direct solutions of the Boltzmann equation [35].

For needles we observe and investigate the breakdown of homogeneity in simulations of dense systems, where the inter-particle spacing is smaller than the length of the needles. Large-scale structures in the translational velocity field are seen to develop. Furthermore the density does not remain homogeneous but clusters form and dissolve again. These effects lead to deviations from the solution of the homogeneous cooling state on the longest times scales and a third stage of cooling is found. It is characterized by an even slower decay of the kinetic energy, most of the energy being stored in the macroscopic velocity field.

We plan to derive generalized hydrodynamic equations for grains with rotational degrees of freedom and in particular hard rods. Such a set of hy-
drodynamic equations could serve as a starting point for a stability analysis, similar to the work of Brito and Ernst [30] for smooth spheres.

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A Calculations for spheres

In this appendix we explain, as an example, the main steps to calculate \( \langle i\mathcal{L}E_{\text{tr}} \rangle_{\text{HCS}} \) of eq. (44) in 2D. We define the configuration integral

\[
Q^N := \int \prod_{i=1}^N dr_i W(r_1, \ldots, r_N) .
\]  

The proper normalized \( N \)-particle distribution function for the HCS-state reads

\[
\rho_{\text{HCS}}(\Gamma; t) = \frac{1}{Q^N W(r_1, \ldots, r_N)} \left( \frac{m}{2\pi T_{\text{tr}}(t)} \right)^N \left( \frac{I}{2\pi T_{\text{rot}}(t)} \right)^{N/2} \exp \left[ -\sum_{i=1}^N \left( \frac{m}{2T_{\text{tr}}(t)} v_i^2 + \frac{I}{2T_{\text{rot}}(t)} \omega_i^2 \right) \right] .
\]  

The angular velocity is a scalar in two dimensions, but a vector in more than two dimensions. Free streaming does not change the energy, so we have to take into account only the collision operator \( \mathcal{L}_+ \) and compute

\[
\langle i\mathcal{L}_+E_{\text{tr}} \rangle_{\text{HCS}} = \frac{1}{2N} \sum_{i \neq j} \int d\Gamma \rho_{\text{HCS}}(\Gamma; t) iT_+^{(ij)} \frac{1}{N} \sum_{k=1}^N \frac{m}{2} v_k^2 =
\]

\[
\frac{1}{2N} \sum_{i \neq j} \int d\Gamma \rho_{\text{HCS}}(\Gamma; t) iT_+^{(ij)} \frac{m}{2} \left( v_i^2 + v_j^2 \right) .
\]

The binary collision operator \( T_+^{(ij)} \) gives a contribution only, if either \( k = i \) or if \( k = j \). Next, we introduce two \( \delta \)-functions,

\[
\langle i\mathcal{L}_+E_{\text{tr}} \rangle_{\text{HCS}} = \frac{1}{2N} \sum_{i \neq j} \int d\Gamma \int dR_1 dR_2 \delta(R_1 - r_i) \delta(R_2 - r_j) \rho_{\text{HCS}}(\Gamma; t) iT_+^{(ij)} \frac{m}{2} \left( v_i^2 + v_j^2 \right) ,
\]  

\( (66) \)
which allows us to replace \( r_i \) by \( R_1 \) and \( r_j \) by \( R_2 \) in \( T_+^{(ij)} \). We define the pair correlation function \( g(|R_1 - R_2|) \) by

\[
\frac{N}{V^2} g(|R_1 - R_2|) := \frac{1}{N(N-1)} \int d\mathbf{r}_k W(r_1, \ldots, r_N) \delta(R_1 - r_i) \delta(R_2 - r_j) .
\]

Equation (67) is used to rewrite eq. (66) in terms of the pair correlation function. Integration over all velocities and angular velocities with index \( k \) and \( i \neq k \neq j \) gives 1 due to normalization. We get

\[
\langle iL_+ E_{\text{tr}} \rangle_{\text{HCS}} = \frac{N}{2V^2} \left( \frac{m}{2\pi T_{\text{tr}}(t)} \right)^2 \int d\omega_1 d\omega_2 d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{v}_1 d\mathbf{v}_2 
\exp \left( -\frac{m}{2T_{\text{tr}}(t)} (\mathbf{v}_1^2 + \mathbf{v}_2^2) - \frac{I}{2T_{\text{rot}}(t)} (\omega_1^2 + \omega_2^2) \right)
\times g(\mathbf{r}) |\mathbf{v}_{12} \cdot \hat{\mathbf{r}}| \Theta (-\mathbf{v}_{12} \cdot \hat{\mathbf{r}}) \delta (|\mathbf{r}| - d) \Delta E_{\text{tr}} .
\]

The loss of translational energy of two colliding particles is denoted by \( \Delta E_{\text{tr}} \). We use the abbreviation \( R_1 - R_2 = \mathbf{r} = r\hat{\mathbf{r}} \) and neglect non contributing terms linear in \( \Omega \) so that \( \Delta E_{\text{tr}} \) is given by

\[
\Delta E_{\text{tr}} = \frac{m}{2} \left[ 2\eta (\eta - 1) (\mathbf{v}_{12}^2 - (\mathbf{v}_{12} \cdot \hat{\mathbf{r}})^2) - (1/2)(1 - e_n^2) (\mathbf{v}_{12} \cdot \hat{\mathbf{r}})^2 + (1/2)\eta_n^2 d^2 (\omega_1 + \omega_2)^2 \right] .
\]

To perform the remaining integrations we substitute

\[
\begin{align*}
\Omega &= \frac{1}{\sqrt{2}} (\omega_1 + \omega_2), & \omega &= \frac{1}{\sqrt{2}} (\omega_1 - \omega_2), \\
V &= \frac{1}{\sqrt{2}} (\mathbf{v}_1 + \mathbf{v}_2), & \mathbf{v} &= \frac{1}{\sqrt{2}} (\mathbf{v}_1 - \mathbf{v}_2), \\
\mathbf{r} &= R_1 - R_2, & \mathbf{R} &= R_1 .
\end{align*}
\]

The Jacobian determinant for the above transformation is 1. Integration over \( \omega, \mathbf{V} \) and \( \mathbf{R} \) all give the value 1 due to normalization. We are left with

\[
\langle iL_+ E_{\text{tr}} \rangle_{\text{HCS}} = N \frac{m}{V^2} \left( \frac{2I}{2\pi T_{\text{tr}}(t)} \right) \int d\Omega d\mathbf{r} d\mathbf{v} 
\exp \left( -\frac{mv^2}{2T_{\text{tr}}(t)} - \frac{I\Omega^2}{2T_{\text{rot}}(t)} \right)
\times \frac{m}{2} \left[ 2\eta (\eta - 1) (\mathbf{v}^2 - (\mathbf{v} \cdot \hat{\mathbf{r}})^2) - (1/2)(1 - e_n^2) (\mathbf{v} \cdot \hat{\mathbf{r}})^2 + (1/2)\eta_n^2 d^2 \Omega^2 \right] .
\]
The integration over $|r|$ yields $dg(d)$. Choosing e.g. $r$ to point along the $x$-axis, the integrals over linear and angular velocities can easily be done as moments of a Gaussian distribution. The result is independent of $\hat{r}$, so that the integration over $\hat{r}$ gives $2\pi$. Finally we obtain the result of eq. (46).

B Calculations for needles

In this appendix we present some of the detailed calculations for needles. As a first step we express the orientation of the rods in spherical coordinates $u_i = (\sin(\theta_i) \cos(\phi_i), \sin(\theta_i) \sin(\phi_i), \cos(\theta_i))$. The canonical momenta (translational and rotational) are then given by

$$p_i = m v_i, \quad p_{\theta_i} = I \dot{\theta}_i, \quad p_{\phi_i} = I \dot{\phi}_i \sin^2 \theta.$$ (73)

In the following calculation it will be necessary to express $\dot{u}_i$ in terms of canonical momenta

$$\dot{u}_i = \frac{p_{\theta_i}}{I} e_{\theta_i} + \frac{p_{\phi_i}}{\sin \theta_i I} e_{\phi_i}.$$ (74)

e$_{\theta_i}$ and e$_{\phi_i}$ are orthogonal unit vectors in $\theta_i$ and $\phi_i$ direction.

The kinetic energies per particle are then given by

$$E_{tr} = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2m} p_i^2, \quad E_{rot} = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2I} p_{\theta_i}^2 + \frac{1}{2I \sin^2 \theta_i} p_{\phi_i}^2.$$ (75)

We want to calculate non-equilibrium expectation values with the normalized probability distribution given in eq. (43). We consider again as an example the translation energy per particle $E_{tr}$.

$$\langle i \mathcal{L} \cdot E_{tr} \rangle = \frac{1}{V^N} \frac{1}{(4\pi)^N} \frac{1}{(2\pi MT_{trans})^{3N/2}} \frac{1}{(2\pi IT_{rot})^N} \frac{1}{2} \sum_{m \neq n} \int \prod_{j=1}^{N} dr_j d\phi_j d\theta_j dp_j dp_{\theta_j} dp_{\phi_j} \exp[-NE_{tr}/T_{tr}(t) - NE_{rot}/T_{rot}(t)] i \mathcal{T}^{(nm)}_{\downarrow} E_{tr}.$$ (76)

Similar to the calculation for the spheres we see that the binary collision operator $\mathcal{T}^{(nm)}_{\downarrow}$ gives a contribution only, if either $i = n$ or if $i = m$. We can sum over $N(N-1)$ identical integrals and get

$$\frac{N-1}{2V^2} \frac{1}{(4\pi)^2} \frac{1}{(2\pi m T_{tr})^3} \frac{1}{(2\pi IT_{rot})^2} \int \prod_{j=1}^{2} dr_j d\phi_j d\theta_j dp_j dp_{\theta_j} dp_{\phi_j} \exp[-E_{tr}^{12}/T_{tr}(t) - E_{rot}^{12}/T_{rot}(t)] \left| \frac{d}{dt} \mid r_{12}^+ \right| \Theta(-\frac{d}{dt} \mid r_{12}^+) \Theta(L/2 - |s_{12}|) \Theta(L/2 - |s_{21}|) \delta(|r_{12}^-| - 0^+) \Delta E_{tr}^{12}.$$ (77)
$E_{12}^{tr}$ ($E_{12}^{rot}$) is the sum of the translational (rotational) kinetic energy of particle 1 and 2 and with $\Delta E_{12}^{tr}$ we denote the change of the translational kinetic energy of particle 1 and 2 in a collision:

$$\Delta E_{12}^{tr} = \frac{(p_1 - p_2) \cdot \Delta p}{m} + \frac{\Delta p^2}{m}, \quad (78)$$

$$\Delta p = -\frac{1 + e_n}{2} \frac{1}{\sqrt{1 + \frac{s_1^2}{4} + \frac{s_2^2}{4}}} (V \cdot u_\perp) u_\perp. \quad (79)$$

$V$ is the relative velocity of the contact points defined in eq. (1).

We introduce relative coordinates $r_{12} = r_1 - r_2$ and $r = r_1$ and the variables

$$z := r_{12} \cdot u_\perp,$$

$$a := r_{12} \cdot u_1 - \frac{u_1 \cdot u_2}{\sqrt{1 - (u_1 \cdot u_2)^2}} r_{12} \cdot u_1^\perp = -s_{12},$$

$$b := \frac{1}{\sqrt{1 - (u_1 \cdot u_2)^2}} r_{12} \cdot u_2^\perp = s_{21}.$$

The Jacobian of the transformation is given by $\sqrt{1 - (u_1 \cdot u_2)^2}$. We remark that $\frac{d}{dt} |r_{12}| = V \cdot u_\perp \text{sign}(r_{12} \cdot u_\perp)$ and we find again the relative velocity of the contact points $V = \frac{m}{z} - a u_1 - b u_2$ given in the new coordinates. Integration over $r$ gives $V$ and integration over $z$ gives the sum of two $\Theta$-functions $\Theta(\pm V \cdot u_\perp)$. This reflects the fact that if one particle touches the other from ‘above’ the sign of the relative velocity of the contact point has to be negative, if the particle touches from ‘below’ the velocity has to be positive. Next one introduces relative and center of mass momenta as well as dimensionless variables:

$$\chi := \frac{1}{\sqrt{2mT_{trans}}} (p_1 - p_2), \quad \gamma := \frac{1}{\sqrt{2mT_{trans}}} (p_1 + p_2),$$

$$\tilde{p}_{\theta_1} := \frac{p_{\theta_1}}{\sqrt{T_{rot}}}, \quad \tilde{p}_{\phi_i} := \frac{p_{\phi_i}}{\sqrt{T_{rot} \sin \theta_i}}.$$

The integration over $\gamma$ can be done and the result is proportional to

$$\sum_{p=\pm 1} \int da \, db \, d\phi_1 \sin \theta_1 \, d\phi_2 \, d\theta_2 \, d\chi \, d\tilde{p}_{\theta_1} \, d\tilde{p}_{\phi_1} \, d\tilde{p}_{\theta_2} \, d\tilde{p}_{\phi_2}$$

$$\frac{1}{\sqrt{1 - (u_1 \cdot u_2)^2}} \exp\left[-\frac{1}{2}(\chi^2 + \tilde{p}_{\phi_1}^2 + \tilde{p}_{\phi_2}^2 + \tilde{p}_{\theta_1}^2 + \tilde{p}_{\theta_2}^2)\right]$$

$$\left|\tilde{V} \cdot u_\perp\right| \Theta \left(p \left|\tilde{V} \cdot u_\perp\right|\right) \Theta(|a| - L/2) \Theta(|b| - L/2) \Delta E_{12}, \quad (80)$$

all expressed in new variables and $\tilde{u}$ by eq. (74), e.g.

$$\tilde{V} = \sqrt{2T_{trans}/m} \chi - a \sqrt{T_{rot}/I} (\tilde{p}_{\theta_1} e_{\theta_1} + \tilde{p}_{\phi_1} e_{\phi_1}) -$$

$$b \sqrt{T_{rot}/I} (\tilde{p}_{\theta_2} e_{\theta_2} + \tilde{p}_{\phi_2} e_{\phi_2}). \quad (81)$$
We want to perform the remaining Gaussian integrals, but we have expressed different terms either in \((u_i^+, u_i^-)\) defined according to eq. (17) with \(i = 1, 2\) or in \((e_{\theta_i}, e_{\phi_i})\). It is useful to note that \((u_i^+, u_i^-)\) and \((e_{\theta_i}, e_{\phi_i})\) are two different orthonormal basis of the plane perpendicular to \(u_i\), so that we can make a orthogonal coordinate transformation from one system to the other. The variables \(\tilde{p}_{\theta_i} = \tilde{v}_{\theta_i} + \tilde{v}_{\phi_i} e_{\phi_i}\) as \(v_i u_i^+ + w_i u_i^-\) with standard normally distributed \(v_i\) and \(w_i\). With this definition of \(v_i\) and \(w_i\) we are able to evaluate for example terms of the form \((\tilde{p}_{\theta_i}, e_{\theta_i}, \tilde{p}_{\phi_i} e_{\phi_i}) \cdot u_\perp = (v_i u_i^+ + w_i u_i^-) \cdot u_\perp = w_1\), where we used \(u_1^+ \cdot u_\perp = u_2^z \cdot u_\perp = 0\). We can integrate freely over \(v_1\) and \(v_2\) and the two components of \(\chi\) perpendicular to \(u_\perp\). We denote with \(d\Omega_i := d\phi_i \sin(\theta_i) d\theta_i\) and the intermediate result reads

\[
\sum_{p=\pm 1} \frac{N-1}{2V} \frac{1}{(4\pi)^2} \frac{1}{(2\pi)^{\frac{3}{2}}} \int da \, db \, ds \, d\Omega_1 d\Omega_2 \exp\left(-\frac{1}{2} s^2\right) \sqrt{1 - (u_1 \cdot u_2)^2} |G \cdot s| \Theta(p G \cdot s) \left[ -s_1 \sqrt{\frac{2\pi}{m}} \frac{1 + e_n}{2} \frac{1}{\frac{1}{m} + \frac{a_i}{2\pi} + \frac{b_i}{2\pi}} G \cdot s + \frac{1}{m} \left(\frac{1 + e_n}{2}\right)^2 \left(\frac{1}{\frac{1}{m} + \frac{a_i}{2\pi} + \frac{b_i}{2\pi}}\right)^2 (G \cdot s)^2 \right]. \tag{82}
\]

We introduced the vectors \(s := (s_1, s_2, s_3) := (\chi \cdot u_\perp, w_1, w_2)\) and \(G = \left(\sqrt{\frac{2\pi}{m}}, -a \sqrt{\frac{2\pi}{m}}, -b \sqrt{\frac{2\pi}{m}}\right)\).

We can now perform the integral over \(s\). We sketch here only how this is done. We want to integrate

\[
\int ds \, \exp\left(-\frac{1}{2} s^2\right) \Theta(\pm G \cdot s) |G \cdot s| |G \cdot s| s_1 . \tag{83}
\]

Let \((e_1, e_2, e_3)\) be the original coordinate system and we define a coordinate system \((e_x, e_y, e_z)\) in which the \(z\)-axis is parallel to \(G\) and we decompose \(s\) in this coordinate system \(s = (s_x, s_y, s_z)\). Then eq. (83) reads

\[
\int ds_x ds_y ds_z \exp\left(-\frac{1}{2} (s_x^2 + s_y^2 + s_z^2)\right) \Theta(\pm s_z) |G| |s_z| [s_x e_x + s_y e_y + s_z e_z] \cdot e_1 . \tag{84}
\]

Only the term, which is proportional to \(s_z e_z\), contributes and the Gaussian integral can easily be performed. Using that \(|G| e_z = G\) we write \(|G| e_z \cdot e_1 = G \cdot e_1 = G\) and we end up with the result \(4\pi |G| G_1\). Only the integrals over \(\Omega_1\) and \(\Omega_2\) have to be done with standard techniques. All other integrals are performed similarly and the results are quoted in the main text.
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