Hydrodynamic theory for dissipative hard spheres with multi-particle interactions

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Extension to kinetic theory and hydrodynamic models are proposed that account for the existence of multi-particle contacts. In the presence of multi-particle contacts (involving elastic, reversible, potential contact energy), dissipation of the translational (kinetic) energy is reduced and a class of different models lead to deviations from the classical inelastic hard sphere (IHS) homogeneous cooling state (HCS), as examined here. The theoretical results are found to be in perfect agreement with the numerical simulations.

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Kinetic theory and the related hydrodynamic models are helpful tools for the modeling and understanding of transport processes in classical, elastic gases for low and moderate densities. The hard sphere (HS) model is the corresponding approach to be implemented as a numerical model. A successful theoretical approach in the spirit of Boltzmann or Chapman and Enskog requires the basic assumptions: (i) The collisions are instantaneous and (ii) subsequent collisions are uncorrelated (“molecular chaos”). Conditions (i) and (ii) lead to the Boltzmann equation, and in the equilibrium state, the velocity distribution is a Maxwellian.

When dissipation is added, one has the inelastic hard sphere (IHS) model, where the coefficient of restitution quantifies dissipation, elastic systems have \( r = 1 \), and \( 1 - r^2 > 0 \) determines the amount of energy lost in a two-particle collision in the center of mass system. The range of applicability of the theory for the IHS was addressed in several papers. However, this is far from the scope of this study, since it involves e.g. Sonine polynomial expansions and “viscoelastic” material behavior, so that we just assume (i–iii) valid for the sake of simplicity.

In this study we restrict ourselves to the homogeneous cooling state (HCS) and focus on a mean-field hydrodynamic approach, neglecting spatial structures like clusters or shear modes. This idealization is reasonable for either weak dissipation, low density or small system size, however, we do not discuss the range of applicability here. The qualitative prediction for the long-time decay of energy with time by Haff is confirmed and it was shown that the distribution function is isotropic in velocity space and it is close to a Maxwellian as long as the system is homogeneous.

In the IHS collisions are always instantaneous, see condition (i), due to the rigid interaction potential. On the first glance, this makes the model (and kinetic theory too) inadequate for the description of real materials for which the interaction potential may be steep, but is perfectly rigid, see Fig. 1. During the contact of two real particles, kinetic energy is stored in elastic (reversible) potential energy that, in the static limit, can be recovered after very long times. The conclusion is thus that one has a fraction of elastic energy, which cannot be dissipated, in the real system. This fraction is missing in all idealized models HS, IHS, and also in the kinetic theory, and has to be defined. Thus we will propose and examine possible ways to cure this problem of the hard sphere model, but keeping kinetic theory still applicable.

![FIG. 1: Schematic plot of the trajectories of two soft (left) and two hard (right) particles against time. The beginning and the ending of the interaction are marked by dashed and dotted vertical lines, respectively, and the time \( t_c \) during that kinetic energy is stored as elastic energy in the contact - so that dissipation is affected - is marked as shaded region.](image-url)

The first step is to define or identify possible multi-particle contacts. In a real system (or in a soft-particle model) one just counts the number of contacts a particle has. Within the extented IHS model, a particle remembers its last contact and every contact occurring within a time \( t_c \) after that, see the shaded area in Fig. 1, is defined a multi-particle contact.

In low density systems, where the mean free flight time is much larger than the contact duration, multi-particle contacts are rare. However, assumption (i) can also be valid in high density situations where the free path is much smaller than the particle diameter: This is possible in the case of an extremely short contact duration, when collisions remain practically instantaneous. Thus we conclude that the free path, i.e. the density, is not an appropriate measure for the occurrence of multi-particle interactions.
contacts. We rather define, as a more objective criterion, the ratio \( \tau_c = t_c/t_E \) between the contact duration \( t_c \) and the typical time between collisions \( t_E \) as obtained by the Enskog theory \([1,7,15]\). Small and large \( \tau_c \) values correspond to pair- and multi-particle collisions, respectively, in our framework \([16]\).

Up to now, the elastic HS model is not changed at all concerning particle trajectories or whatsoever. The only modification is, that every particle that had a collision a short time ago keeps this event in memory for the contact duration \( t_c \) and every new contact occurring within this time is now defined as an elastic contact. This allows to split the total energy in the system into a kinetic and an elastic (potential) contact energy \([16]\), as can be done in a real system. If a part of the kinetic energy is transferred to contact energy, it cannot be dissipated anymore, so that energy dissipation in the IHS model has to be reduced in the presence of multi-particle contacts. This qualitative reduction of energy dissipation in dense systems has been observed in soft-particle molecular dynamics simulations \([17]\).

Recently, the transition of a granular gas to its solid counterpart has been investigated \([15,18]\). A general model was defined, in which the coefficient of the normal restitution is given by

\[
r = r(x) = \begin{cases} 
  r_0, & \text{if } x > x_c \\
  1, & \text{if } x \leq x_c \end{cases}
\]  

with the dimensionless time \( \tau = (2/3)At/t_E(0) \), scaled by \( A = (1 - r^2)/4 \), and the initial collision rate \( t_E(0) \). In these units, the energy dissipation rate \( I \) is a function of the dimensionless energy \( E = K/K(0) \) with the kinetic energy \( K \), and the cut-off parameter \( x_c \). In this representation, the restitution coefficient is hidden in the rescaled time via \( A \), so that IHS simulations with different \( r \) scale on the master-curve in the following plots. In the following, we will extract the classical dissipation rate \( E^{3/2} \) \([12]\) from \( I \), so that

\[
I(E, x_c) = J(E, x_c) E^{3/2},
\]  

where \( J \) is the correction-function \( J \rightarrow 1 \) for \( x_c \rightarrow 0 \). Our theoretical results will be compared with numerical simulations and with previous results \([16]\). For the derivation of the dimensionless equation \((2)\) from the kinetic theory in its dimensional form, see Refs. \([14,23]\).

For the classical IHS model in the HCS, Eq. \((2)\) is solved by \( E_r = (1 + x)^{-2} \), a master curve, independent of the coefficient of restitution \( r \) and all other system parameters. We checked via simulations that different \( r \) values scale on the same master-curve, as long as no clustering is obtained. We will proceed to develop our theory in the dimensionless variables and will examine in detail the deviations from the classical HCS.

The velocity cut-off (VC) model can be rationalized based on the picture of elasto-plastic particles which do not suffer inelastic (plastic) deformation if they collide below a certain threshold velocity \( v_c \). In static contact, the relative velocity vanishes and thus is automatically smaller than \( v_c \), see \([14]\) for a recent application. The deviation from the classical inelastic hard sphere HCS,

\[
J(E, v_c) = (1 + \xi^2) \exp \left( -\xi^2 \right),
\]  

is obtained from the (cumbersome) computation of the collision integral \([18]\), with the nondimensional quantity

\[
\xi^2 = \frac{3mv_c^2}{8K(1)} = \left( \frac{v_c^2}{4v_F^2} \right) = \frac{V_c^2}{E} \propto E^{-1},
\]  

which relates the critical velocity to the actual mean fluctuation velocity. The dimensionless cut-off velocity is \( V_c = v_c/2v_F(0) \). For \( v_c = 0 \) and thus \( \xi = 0 \), the classical homogeneous cooling state is recovered, i.e., \( J(E, 0) = 1 \).

Event driven numerical simulations \([1,10]\) are compared to the numerical solution of our theory in Fig. \([3]\). We obtain perfect agreement between theory and simulations in the examined range of \( v_c \)-values. The fixed cut-off velocity has no effect when the collision velocities are very large, \( v_F \gg v_c \), but strongly reduces dissipation when the relative velocity at collision is comparable to or smaller than \( v_c \). Thus, in the homogeneous cooling state, there is no effect initially, but the long time behavior changes from the classical decay \( E \propto t^{-2} \) to a
The free path cut-off (LC) model was used first by McNamara and Young \cite{19} to avoid the inelastic collapse, and was extended to its simple hydrodynamalogon expressed in terms of the density by Kamenetsky et al. \cite{22,23} to describe the gas solid transition caused by the compression of a granular gas. The physical idea is that particles that are near to each other – their distance is below a certain threshold which can be regarded as some surface roughness – are supposed to be in contact with each other, so that their contact potential energy cannot be dissipated.

The deviation from the classical inelastic hard sphere HCS is $J(E, \tau_c) = J(\tau_c) \propto E^0$, a constant independent of the energy and thus independent of time. Thorough calculation \cite{18} yields

$$J(\tau_c) = \exp(-k \varepsilon_\lambda),$$

with $\varepsilon_\lambda = \lambda_c (N/V) (4a)^2 g_{2a}(\nu) = \lambda_c / \sqrt{\pi} \lambda$, and constant $k \approx 7.37$. This result can be understood, since in the homogeneous cooling regime, one has constant density and thus constant mean free path, so that a free path cut-off model has a time independent effect. Due to its lack of interesting new phenomena for the HCS, we will not discuss the LC model further.

The TC model was invented in order to model elastic material properties, like the “detachment” effect \cite{17}, in the framework of the IHS model. In soft assemblies of particles this resembles multi-particle contacts and avoids the inelastic collapse in dense IHS systems \cite{16,24,25}; the physical idea behind was discussed in the introduction. In technical terms, a collision is elastic if any one of two colliding particles had a collision within a time $t_c$ before the actual time.

The deviation from the classical HCS is, see \cite{18},

$$J(E, t_c) = \exp(\Psi(x)), \quad \text{(7)}$$

with the series expansion $\Psi(x) = -1.268x + 0.01682x^2 - 0.0005783x^3 + O(x^4)$ in the collision integral, with $x = \sqrt{\pi} \tau_c t_E^{-1}(0) \sqrt{E} = \sqrt{\pi} \tau_c(0) \sqrt{E} = \sqrt{\pi} \tau_c$. This is close to the result $\Psi_{LM} = -2x/\sqrt{\pi}$, proposed by Luding and McNamara, based on probabilistic mean-field arguments \cite{10,26}. Here, the argument of the exponential is proportional to the collision rate $t^{-1} \propto \sqrt{E}$, different from the other models, so that $J \propto \exp(\sqrt{E})$.

Simulation results are compared to the theory in Fig. 3. The agreement between simulations and theory is almost perfect in the examined range of $t_c$-values, only for large deviations from the HCS solution and for large $t_c$-values, a few percent discrepancy are observed \cite{29}.

The results can be explained as follows. The fixed cut-off time has no effect when the time between collisions is very large $t_E \gg t_c$, but strongly reduces dissipation when the collisions occur with high frequency $t_E^{-1} \gtrsim t_c^{-1}$. Thus, in the homogeneous cooling state, there is a strong effect initially, but the long time behavior tends towards the classical decay $E \propto t^{-2}$.

Additional simulations with a set of system-sizes and for different (also very small) restitution coefficients will be discussed elsewhere \cite{14}. Note however, that our conclusions are valid for all system sizes examined and for arbitrary restitution coefficients before the inhomogeneities evolve.

In summary, a general class of cut-off models was presented, aiming towards the enhancement of classical kinetic theory with respect to the realistic behavior of dissipative particles in the presence of multi-particle interactions \cite{23}. Analytical expressions for the collisional cooling rate in the energy balance equation of the hydrodynamic equation is provided for the multi-particle contacts, evading the singularity of the inelastic collapse. Our theoretical results were verified by event-driven numerical simulations of the HCS and perfect agreement was obtained. For realistic material behavior combinations of the models and also refinements may be necessary. Our model, however, leads to a correction of the energy dissipation term alone, in the framework of a hydrodynamic continuum theory. We regard it thus as much simpler than the model proposed in Ref. \cite{20} that also takes the finite contact duration into account.

The TC model, and to some extent also the other models, are based on the assumption that the elastic, reversible, potential contact energy of real particles cannot be dissipated in the same way as the kinetic energy. If one has multi-particle contacts in the system, a lot of energy is stored in their contacts – and thus cannot be dissipated.
FIG. 3: Deviation from the HCS, i.e. rescaled energy $E/E_r$, plotted against $\tau$ for simulations with different $\tau_c(0)$ as given in the inset, with $r_0 = 0.99$, and $N = 8000$. Symbols are simulation results, the dashed line is the first order correction, the solid line results from the third order, and the dotted line correspond to the results from $[16]$.

Future interesting work could be the extension of our cut-off models to more complicated material laws, e.g., introducing some velocity dependent restitution coefficient $r(v)$ or contact duration $t_c(v)$. In the same spirit, the cut-off law can be replaced by continuous functions instead of step-functions $[31]$. In addition, the present theory should be applied to hydrodynamic models of in-homogeneous systems, where the cut-off criterion is a function of the position, in order to prove its general applicability. As another verification, the model could be compared to soft-sphere simulations and experiments.

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[27] This simplification also is reasonable in the spirit and the framework of the kinetic theory and numerical event-driven simulations, where changes of the particle velocities occur as instantaneous, discontinuous events
[28] $\Psi_{LM}$ thus neglects non-linear terms and underestimates the linear part
[29] The simulation has to be carefully prepared for the TC model in order to achieve good agreement. First, the system is relaxed elastically with $r = 1$ for several hundred collisions per particle and the last time of collision is saved for each particle. Second, the dissipation is switched on and the TC model is activated using the saved information about previous contacts. If this information is not used, one observes an artificial initial decay of energy in the simulation.
[30] Only the TC model was used for the detailed discussion
[31] However, since experimental data are missing, we prefer the simple event-based model which is consistent with the kinetic theory