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Collisional cooling with multi-particle interactions

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Abstract An extension to kinetic theory and hydrodynamic models is proposed that accounts for the existence of multi-particle contacts and leads to a correction of the cooling rate. The other hydrodynamic terms remain unchanged. In the presence of multi-particle contacts a class of different models leads to deviations from the classical inelastic hard sphere (IHS) results. For the homogeneous cooling state (HCS), as examined here, the theoretical results are found to be in perfect agreement with the numerical simulations.
Keywords: Hard spheres, multi-particle contacts, kinetic & hydrodynamic theory, contact duration, TC model

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 [1, 2]. The hard sphere (HS) model is the corresponding approach to be implemented as a numerical model [3, 4]. A successful theoretical approach in the spirit of Boltzmann or Chapman and Enskog [1, 2] 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 (iii) a Maxwellian.

When dissipation is added, one has the inelastic hard sphere (IHS) model, where the coefficient of restitution r 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 [5–8]; here we just assume that (i–iii) are approximately 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 [5–7, 9–11], neglecting spatial structures like clusters or shear modes. This idealization is reasonable for either weak dissipation, low density or small system size. The qualitative prediction for the long-time decay of energy by Haff [12] 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 [8, 13, 14].

In the IHS model 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 *never* 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 the total energy, i.e. the elastic energy, *which is not 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.

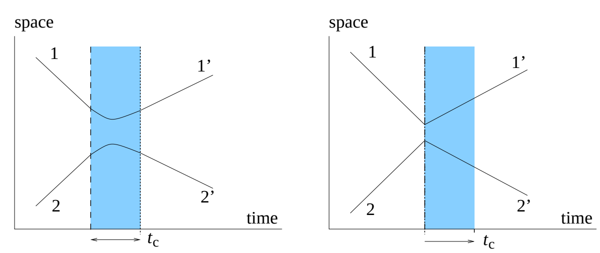

Fig. 1. Schematic plot of the trajectories of two soft (left) and two hard (right) particles against time. The beginning and the ending of the interaction are marked by dashed and dotted vertical lines, respectively, and the time t_c during that kinetic energy is stored as elastic energy in the contact is marked as shaded region. In the left figure it corresponds to the contact duration, in the right figure it is a memory time of hard spheres, similar in magnitude, with the same meaning "contact duration".

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. A new contact occuring within a time t_c

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after that, see the shaded area in Fig. 1, is thus a multi-particle contact. The memory time t_c is referred to as "contact duration" in the following.

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 occurence of multi-particle 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 τ_c values correspond to pair- and multi-particle collisions, respectively, in our framework [15].

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 occuring 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], like in a real system. If a part of the kinetic energy is transfered 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]. The initial configuration of the simulation has thus to account for the history, back t_c in time.

Recently, the transition of a granular gas to its solid counterpart has been investigated [16, 18]. A general model was defined, in which the coefficient of the normal restitution is given by

$$r = r(x) = \begin{cases} r_0 \,, & \text{if} \quad x > x_c \\ 1 \,, & \text{if} \quad x \le x_c \end{cases} \qquad (1)$$

where x is a variable and x_c is the respective cut-off value. Above the threshold, one has the usual inelastic hard sphere mode with constant restitution coefficient, below the cut-off an elastic system with $r = 1$ is assumed. The variables proposed were either the time between collisions (TC model), the distance travelled since the last collision (LC model), or the relative velocity of two particles prior to a collision (VC model). In order to keep the following analysis simple, we focus on the special case of a piecewise constant restitution and disregard any continuous dependency of r on x, a reasonable simplification 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.

Variants of the general model have been used [14, 16, 19–23], mainly to avoid the "inelastic collapse", an artefact of the rigid particle model, which allows an infinite number of collisions to occur within a finite time. In the real system this can never occur due to the fact that the contacts take a finite time so that lasting multi-particle contacts can form. The model in Eq. (1), avoids the inelastic collapse, since the dense parts of the system, where the collapse tends to occur first, are transformed into elastic regions where the inelastic collapse is unlikely. Thus the inelastic collapse is replaced by "static", dense regions of the material: The particles rattle around in their cages with a high collision rate and practically all collisions are elastic.

The different variants of the cut-off model will be discussed separately in the following, because they lead to different forms of the collision integral. The general form of the energy balance equation is

$$\frac{d}{d\tau} E = -2I(E, x_c) \,, \qquad (2)$$

with the dimensionless time $\tau = (2/3)At/t_E(0)$, scaled by $A = (1-r^2)/4$, and the collision rate $t_E^{-1} = \frac{12}{a}\nu g(\nu)\sqrt{\frac{T}{\pi m}}$, with $T = 2K/(3N)$. 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. The classical dissipation rate $E^{3/2}$ [12] is extracted from I, so that

$$I(E, x_c) = J(E, x_c) E^{3/2} \,, \qquad (3)$$

with the correction-function $J \to 1$ for $x_c \to 0$. 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. [16, 23].

For the classical IHS model in the HCS, Eq. (2) is solved by $E_\tau = (1 + \tau)^{-2}$, 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,

$$J(E, v_c) = \left(1 + \xi^2\right) \exp\left(-\xi^2\right) \,, \qquad (4)$$

is obtained from the computation of the collision integral [18], with the nondimensional quantity

$$\xi^2 = \frac{3mv_c^2}{8K(t)} = \left(\frac{v_c^2}{4v_T^2}\right) = \frac{V_c^2}{E} \propto E^{-1} \,, \qquad (5)$$

which relates the critical velocity to the actual mean fluctuation velocity. The dimensionless cut-off velocity is $V_c = v_c/2v_T(0)$. 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 [11, 16] are compared to the numerical solution of our theory in Fig. 2.

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, $v_T \gg v_c$, 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 logarithmic decay as shown below.

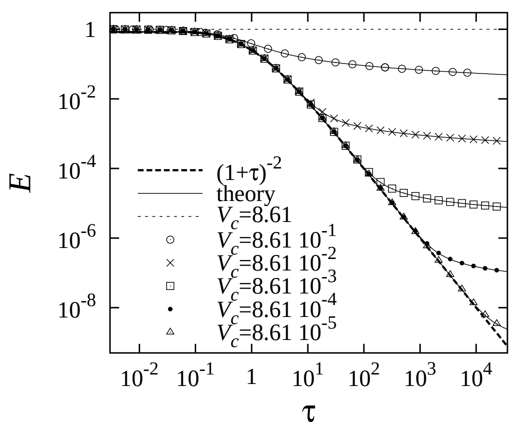

Fig. 2. Energy E plotted against time τ for a simulation with $N = 19683$ particles, density $\nu = 0.08245$, coefficient of restitution $r_0 = 0.99$ and different V_c as given in the inset. The symbols are simulations and the lines give the solution of Eqs. (2,3), using Eqs. (4,5).

In order to understand the long time behavior of the VC model, Eqs. (2), (3), and (4) yield

$$\frac{dy}{d\theta} = y^{3/2}\exp(-y) \ , \qquad (6)$$

after susbtitution $y = V_c^2/E$ and $\theta = 2V_c t$. in the asymptotic limit for $y \gg 1$ and $\theta \gg 1$. The two leading terms of the asymptotic solution of this equation are

$$y = \ln(\theta) + (3/2)\ln(\ln(\theta)) \ . \qquad (7)$$

Finally, combining the leading term of y with the definition, leads to $E \propto V_c^2/\ln(2V_c t)$, a non-trivial logarithmic asymptotic decay of energy, in agreement with the two-dimensional results presented in Ref. [24]. Even when no clusters would occur in the system for large times, we believe it will be quite challenging to find this asymptotic behavior with simulations.

The *free path cut-off (LC) model* was used first by McNamara and Young [19] to avoid the inelastic collapse, and was extended to its simple hydrodynamic analogon expressed in terms of the density by Kamenetsky et al. [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 cut-off length λ_c, 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 $J(E, \lambda_c) = J(\lambda_c) \propto E^0$, a constant independent of the energy and thus independent of time. Thorough calculation [18] yields

$$J(\lambda_c) = \exp(-k\varepsilon_\lambda) \ , \qquad (8)$$

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 [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 [16, 25, 26]; 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 the cumbersome mathematics in Ref. [18],

$$J(E, t_c) = \exp\left(\Psi(x)\right) \ , \qquad (9)$$

with the series expansion $\Psi(x) = -1.268x + 0.01682x^2 - 0.0005783x^3 + \mathcal{O}(x^4)$ in the collision integral, with $x = \sqrt{\pi}t_c t_E^{-1}(0)\sqrt{E} = \sqrt{\pi}\tau_c(0)\sqrt{E} = \sqrt{\pi}\tau_c$ [18]. This is close to the result $\Psi_{\rm LM} = -2x/\sqrt{\pi}$, proposed by Luding and McNamara, based on probabilistic mean-field arguments [16]. Here, the argument of the exponential is proportional to the collision rate $t_E^{-1} \propto \sqrt{E}$, different from the other models, so that $J \propto \exp(-\text{const.}\sqrt{E})$.

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

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 [18]. 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. Only the TC model is discussed in detail below. Analytical expressions for the collisional cooling rate in the energy balance equation of the hydrodynamic equation is provided for the multi-particle contacts, evading

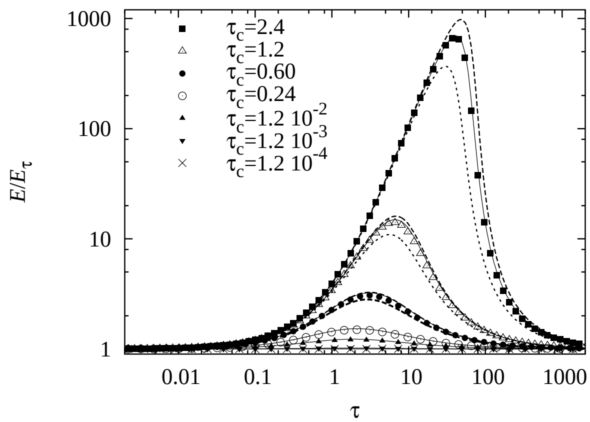

Fig. 3. Deviation from the HCS, i.e. rescaled energy E/E_τ, plotted against τ for simulations with different $\tau_c(0)$ as given in the inset, with $r_0 = 0.99$, and $N = 8000$. Symbols are simulation results, the dashed line is the first order correction, the solid line results from the third order, and the dotted line correspond to the results from [16].

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 neccessary. Our model leads to a correction of the energy dissipation term, in the framework of a hydrodynamic continuum theory. We regard it thus as much simpler than the model proposed in Ref. [27] that also takes the finite contact duration into account, but leads to changes of all hydrodynamic equations.

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.

Future interesting work involves combinations of the models and the extension of the simple 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, however, since experimental data are missing, we prefer the simple event-based model which is consistent with the kinetic theory. In addition, the present theory should be applied to hydrodynamic models of inhomogeneous 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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