Homogeneous Cooling
with Repulsive and Attractive Long-range Interactions

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Abstract. In granular matter, consisting of discrete particles, long-range interactions imply that each of the particles is interacting with all others. For many charged granular materials with Coulomb repulsion or large-scale gravitationally attractive systems, a Molecular Dynamics environment is developed. In granular systems with long-range interaction forces and dissipative collisions, both effects can lead to large-scale structure formation, whereas already dissipation alone leads to ever growing clusters. For our three-dimensional mono-charged dissipative homogeneous systems we present the effect of both repulsive and attractive mutual long-range forces and make an attempt to predict the collision frequency and the temperature decay in the system by means of a modified pseudo-Liouville operator formalism. The theoretical predictions are in perfect agreement with the simulations, but only in the limit of low density and for not too strong interaction potential enrgy.

Keywords: 1/r potentials, Molecular Dynamics, granular gases, pseudo-Liouville operator formalism;
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INTRODUCTION

Treating long-range potentials by computer simulations of discrete particles correctly has always been a challenge in various research fields such as protein folding in aqueous solutions, the evolution of star clusters in astrophysics [1] or simply the collision behavior of electrostatically charged particles [7]. Algorithms have been developed, e.g., [2] in order to encounter these highly specialized problems in a computationally effective way and have also been implemented in discrete element methods such as Molecular Dynamics.

In this study, we perform Molecular Dynamics simulations of dilute homogeneous dissipative particle systems where particles either mutually repel or attract each other via a 1/r-long-range potential [10]. As reference, we make use of the inefficient pair-wise summation, i.e., we sum up the forces of all particles acting on the particle of interest. We then compare the reference with results that are obtained by our new hierarchical cell algorithm that is more efficient regarding the computational time expense. Finally, we develop a theory for long-range binary particle interactions that is based on the so-called pseudo-Liouville operator formalism, e.g., [3] and compare it with our simulation results.

MOLECULAR DYNAMICS

"Short" and "Long"-range Forces

We use soft-sphere Molecular Dynamics where within each time step Newton's equations of motion for each particle are solved by the simple Verlet integration method. For this, all currently acting forces on each particle have to be known. During a collision between particles i and j with radii $a_i = a_j = a$, a linear repulsive force and dissipation of kinetic energy in normal direction, $\boldsymbol{n}_{ij} = \boldsymbol{r}_{ij}/r_{ij} = (\boldsymbol{r}_i - \boldsymbol{r}_j)/|\boldsymbol{r}_i - \boldsymbol{r}_j|$, is considered. The loss of kinetic energy at each collision is expressed by the coefficient of normal restitution $r = v_{ij}^{'(n)}/v_{ij}^{(n)}$ that gives the ratio of the relative velocities v_{ij} in normal direction after (primed) and before (unprimed) the collision. During a time step, on one particle i always long-range forces are acting due to the pair-wise summation,

$$\boldsymbol{F}_i^{(long)} = -Kx^2 \sum_{j=1}^{N-1} \sum_{j=k+1}^{N} \frac{\boldsymbol{n}_{ij}}{r_{ij}^2} \qquad (1)$$

and, if $r_{ij} < 2a$, short-ranged contact forces as well

$$F_i^{(short)} = k(2a - r_{ij})\boldsymbol{n}_{ij} - \gamma_n(\boldsymbol{v}_{ij} \cdot \boldsymbol{n}_{ij})\boldsymbol{n}_{ij} \qquad (2)$$

x denotes here either the charge or mass of particles if we deal with an electrostatic or gravitational problem with mono-charged particles of the same mass. According to the spring-dashpot model [4], γ_n is a measure for how much kinetic energy is dissipated at each collision whereas *k* is the spring constant that defines the stiffness. $K = cG$ defines via *c* (which is positive for repulsive and negative for attractive forces) the strength of the long-range force, where *G* denotes a constant.

Pair-wise Summation

Pair-wise summation computes the distances between each of the *N* particles and all others. The computational time expense then scales with the order of the squared particle number, $O(N^2)$. In presence of short-ranged (contact) potentials only, when particles far from each other do not interact, there is no need to apply the pair-wise summation. In such a case we can reduce the time expense to $O(NM)$ if we check only *M* neighboring particles for collision [5].

In case of long-range potentials, when even particles far from each other do interact via weakly repulsive or attractive potentials, we will apply the expensive pair-wise summation method in order to obtain most accurate results. In the following, we discuss homogeneously distributed mutually short and long-ranged interacting particles in a three dimensional box with periodic boundaries. The implementation of periodic boundaries suppresses box surface effects and keeps the particle system homogeneous during its time evolution.

RESULTS

Pseudo-Liouville Operator Theory

For derivation and explanation of the pseudo-Liouville operator formalism, we refer to [3]. Here, we only will outline this idea briefly.

According to classical mechanics, the total time derivative of a dynamical variable, $A(t)$, of a *N*-body system contains the *Hamiltonian* which represents the total energy of the system and its spatial derivatives. Moreover, the system obeys the Liouville-equation that says that during its time evolution all possible states can be taken with the same probability, i.e., the probability density in phase space is conserved. For

hard sphere systems the interaction potential within the Hamiltonian represents a discontinuous function and problems will arise if we apply spatial derivatives. Therefore, for dissipative hard sphere systems, the pseudo-Liouville operator was introduced in order to bypass these problems and to preserve the formal structure of the Liouville-equation. Although we simulate soft spheres, we can make use of the pseudo-Liouville operator formalism because the soft spheres behave anyway nearly like hard spheres in our simulations besides the effect of strong long-range forces. For dynamical variables that are determined by dissipative particle collisions, the interaction part, L^+, of the pseudo-Liouville operator is used for the total time derivative and selects only those pairs of particles that are in physical contact and neglects all others. The total time derivative expressed by the pseudo-Liouville operator reads

$$\frac{d[A(t)]}{dt} = L^+ A(t) = \sum_{j=1}^{N-1} \sum_{k=j+1}^{N} \left|\boldsymbol{v}_{jk} \cdot \boldsymbol{n}_{jk}\right| \Theta\left(-\boldsymbol{v}_{jk} \cdot \boldsymbol{n}_{jk}\right)$$
$$\times \delta\left(\left|\boldsymbol{r}_{jk}\right| - 2a\right)\left(b_{jk}^+ - 1\right) A(t), \quad (3)$$

where *j* and *k* are two arbitrary particles. The sums go over all particle pairs. $\delta(|\boldsymbol{r}_{jk}|-2a)$ is the delta function that considers only touching particle pairs, i.e., it vanishes if the distance is larger than twice the radius of the particles. $\Theta(-\boldsymbol{v}_{jk} \cdot \boldsymbol{n}_{jk})$ is the step function that selects only those normal velocities between two particles that are negative, i.e., that lead to an approach and, thus, to a collision between both particles if they are in contact. $|\boldsymbol{v}_{jk} \cdot \boldsymbol{n}_{jk}|$ is the normal component of relative velocity and increases the number of collisions per time unit because higher travel speed will lead to more collisions with other particles. (b^+-1) is the binary collision operator that acts on $A(t)$ and changes the velocity and position variables of the particles in $A(t)$ due to the current collision.

Using the collision frequency, $f_E(t)=(2/N)(dC(t)/dt)$, and the (kinetic) energy dissipation rate, $dE_{kin}(t)/dt$, as dynamical variables in Eq. (3), we apply the concept of ensemble averages by using the *N*-body distribution function. $C(t)$ is the total number of collisions in the system so far. Skipping all the formal details containing integrations over all phase space coordinates, we only will provide here the solution. Note, that for the velocity integrations we have to distinguish between the presence and absence of long-range forces, between repulsive and attractive forces. We obtain for the case without long-range potentials

$$f_E^0(t) = 16\sqrt{\pi}na^2 g^0(2a)T_g(t)^{1/2} \qquad (4a)$$

$$I^0(t) = \frac{d[E_{kin}(t)]}{dt} = -8\sqrt{\pi}nNma^2(1-r^2)g^0(2a)T_g(t)^{1/2} \quad (4b)$$

for the case of long-range repulsive potentials

$$f_E(t) = f_E^0(t)\exp\left(-\frac{v_{n,b}^2}{2T_g(t)}\right) \quad (5a)$$

$$I(t) = I^0(t)\exp\left(-\frac{v_{n,b}^2}{2T_g(t)}\right) \quad (5b)$$

and for the case of long-range attractive potentials

$$f_E(t) = f_E^0(t)\left[2 - \exp\left(-\frac{v_{n,e}^2}{2T_g(t)}\right)\right] \quad (6a)$$

$$I(t) = I^0(t)\left[2 - \exp\left(-\frac{v_{n,e}^2}{2T_g(t)}\right)\right] \quad (6b)$$

Here, $v_{n,b} = (2c_bkx^2/(ma))^{1/2}$ is the critical normal relative velocity both particles have to exceed in order to overcome the repulsion potential barrier and collide. On the other hand, the normal relative velocity has to be less than $v_{n,e} = (2c_ekx^2/(ma))^{1/2}$ in order to be caught by the attractive potential and to have a collision. $T_g(t)$ is the granular temperature, m the mass of the mono-dispersed particles, $g^0(2a)$ the pair distribution function for hard spheres at contact that describes the probability to find a neighbor particle exactly at $|r_{jk}| = 2a$ and n denotes the particle number density.
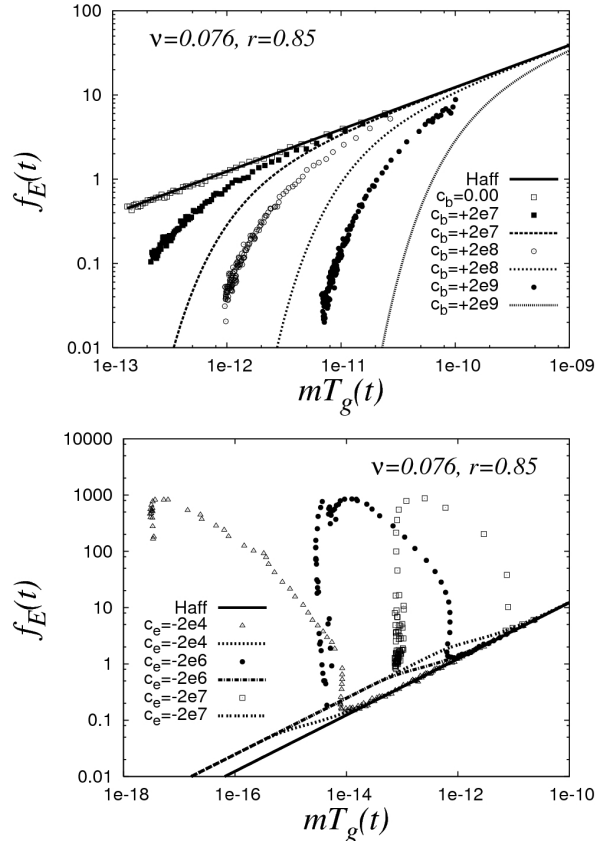
FIGURE 1. Pair-wise summation method applied for repulsive (top) and attractive systems (bottom). $f_E(t)$ is plotted against $mT_g(t)$ for different c_b and c_e.
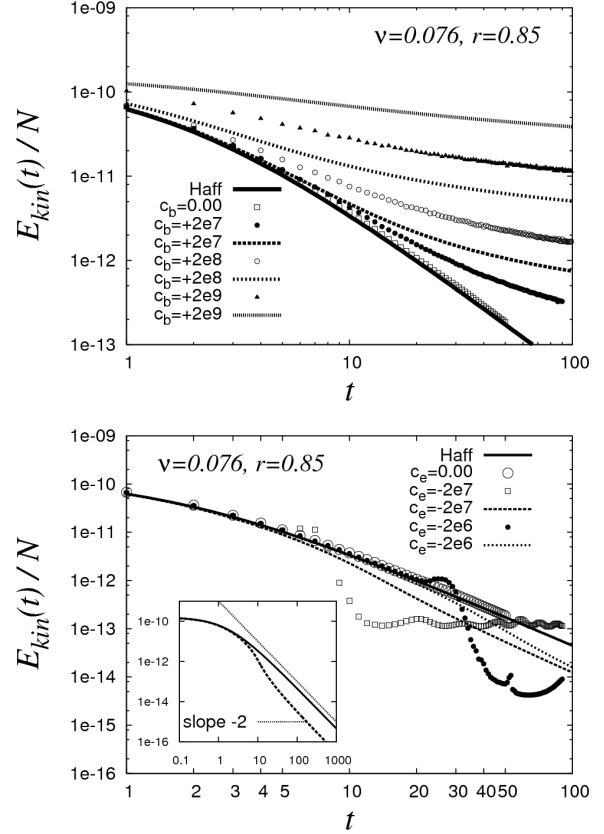
FIGURE 2. Pair-wise summation method applied for repulsive (top) and attractive systems (bottom). $E_{kin}(t)/N$ is plotted against time for different c_b and c_e.

Computer Simulations

In order to compare with theory we used the accurate pair-wise summation method. Fig. 1 shows the collision frequency, $f_E(t)$, plotted against the system's temperature for both the repulsive (top) and attractive case (bottom panel) in a double logarithmic plot. $f_E(t)$ decreases because the system cools down due to dissipative collisions ($r = 0.85$). For different potentials, the simulation results are compared with Eqs. (5a) and (6a). In both cases, for high temperatures in the beginning, the equations and the data approach the classical results, expressed by Eq. (4a) and Haff's law (4b) [9]. For low temperatures, the interaction potential becomes important and deviations from Haff's law occur. For repulsive particles there are also deviations between theory and simulation because theory does not take many body effects into account. The many-body effect is responsible for small deviations between theory and simulation but discussed in [10]. In the attractive case, theory

indicates pretty well the point when the collision rate increases rapidly and the system becomes strongly inhomogeneous. This corresponds to the hump in $E_{\text{kin}}(t)$ shown in Fig. 2 (bottom) where the particles are close to each other and have higher kinetic energy due to the higher attractive forces. The solutions of Eqs. (5b) and (6b) are also shown in Fig. 2. Here, due to the many-body effect, theory qualitatively predicts the simulation data, where for high temperatures both theory and data approach the classical result (4a) and (4b) whereas for low temperatures, deviations between $E_{\text{kin}}(t)$ and the classical result occur as well.

CONCLUSIONS

We used the pseudo-Liouville operator formalism that is a two-particle theory for hard spheres, extended it for both repulsive and attractive long-range interactions and applied it to our simulation results. It turned out that for repulsive forces theory approaches the results reported in Ref. [7]. For attractive forces it successfully predicts when the transition between the homogeneous and inhomogeneous regime takes place. Additionally, in the limit $T_g(t) >> v_{n,b/e}^2$ it contains the classical results as required.

The discrepancies between theory and simulation in the repulsive case result from the fact that the pseudo-Liouville theory is a two-particle theory that perfectly works only for systems in the dilute limit. We lack of an analytical prediction for systems with high densities where many-particle effects become important. Anyway, a good agreement in theory and simulation is achieved when we simulate systems with very low density [10].

OUTLOOK

An interesting task will be the analytical prediction of the cooling behavior of repulsive and attractive systems at moderate and high densities. At this moment we are not able to meet this challenge, but we already have approached this aim in an empirical way. In [10] an empirically developed, density-dependent correction to Eqs. (5a)-(6b) was proposed, using data from finite density simulations.

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