Statistical Mechanics of Granular Systems

by

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Abstract

From a first principles theory for the behavior of smooth granular systems, we derive the form for the instantaneous dissipative force acting between two grains. The present model, which is based on the classical harmonic crystal, reproduces the dependence of the kinetic energy dissipation on the grain deformation obtained by models that assume a viscoelastic behavior (without permanent plastic deformations) during the collision.

We then derive kinetic equations for the rarified granular gas from the Fokker-Planck equation that describes the time evolution of the reduced distribution function for the translational granular degrees of freedom. We obtain the inelastic dissipation rate term and calculate the time evolution of the granular temperature for the homogeneous granular gas. We also derive kinetic equations for the non-homogeneous, rarified granular gas and obtain hydrodynamic equations for the system.

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Contents

Chapter 1

Introduction

1.1 What are granular systems?

Granular systems (GS) are one of the most interesting forms of organization of matter[1]. They are large conglomerates of discrete macroscopic particles. They are present, in many ways, in our day-to-day lives: in industrial applications, geological phenomena, in a stroll at the beach.

One of the characteristics that makes GS special, is the fact that they possess a very large number of internal degrees of freedom. In fact, this is basically what distinguishes GS from molecular systems [2]. Their presence makes a single grain behave as a thermal bath by itself. It is thus impossible to keep track of the internal degrees of freedom in an exact way. Averaging procedures that eliminate the redundant fast degrees of freedom will be necessary in order to understand the behavior of these systems[3]. The consequence is that some information is irreversibly lost when grains interact. This is the cause of inelasticity in granular collisions. Friction and the excluded volume (due to the repulsive hard core of the grains) play a fundamental role in the way GS organize themselves[1]. That arrangement is determined by gravitation and the boundary conditions on the system. For instance, a sand pile that lies on a horizontal table (static case) behaves quite differently from one in which that same table is tilted at some large angle (flow, dynamic case). For dry granular systems, intersticial fluids, such as air, can be neglected for most of the flow or static properties of system[4].

A remarkable characteristic of these systems is that the internal (or thermodynamic) temperature T, is basically irrelevant for the dynamical behavior of the system[5]. The typical granular kinetic energy is many times larger (10^{12} is a typical value for grains of sand in flow) than $k_B T$. This limits severely the phase-space sampling ability of GS. After the dissipative dynamical relaxation, most of the kinetic granular energy is lost and the grains can get "stuck" in a given configuration indefinitely.

1.2 The problem

In the present work, we want to analyze the flow properties of classical GS. The reason to use a classical approach for treating GS is that the de Broglie wavelength for these systems is completely negligible compared with the physical lengths of the problem.

Our goal is then to derive kinetic and hydrodynamic equations of motion that describe the behavior of GS in the regimes of low density and small gradients. These limitations are imposed upon us primarily by the complexity of the task, in the sense that we need to make expansions and truncations on the original Liouvillian problem with the help of small parameters of the theory (density & gradients)[6].

The flow properties of GS are unusual from the point of view of simple molecular fluids. In general, motion occurs in segregated laminar layers, needing strong external perturbations in order to excite bulk motion[7]. We are interested in finding a description for the fluidised rarified phase.

As a brief summary, in chapter 2, we will study the granular collision and the viscoelastic kinetic energy dissipation mechanism, for a system of identical, smooth and spherical granular particles. In chapter 3, we develop the mathematical techniques necessary to obtain the kinetic or hydrodynamic equations for GS in the regime of low density and small gradients. In chapter 4, we study the homogeneous granular gas and the time dependence of the granular temperature (defined as the average kinetic energy of a grain). In chapter 5, we study the hydrodynamic behavior of the non-homogeneous granular gas (GG).

1.3 Granular collisions

As stated above, kinetic energy is dissipated in an irreversible manner via the excitation of internal vibrational modes during a collision[12]. These modes act like an ideal sink of energy, given that the number of internal degrees of freedom is vast. They are capable of absorbing a large amount of thermal energy without any appreciable increase in their internal temperature, T.

There are several mechanisms of relaxation of the internal degrees of freedom. The most important for us being the viscoelastic[9, 10] and the plastic[11] mechanisms (others are: crack formation and propagation[8], elastic vibration of the grains, sound wave excitation on the surrounding fluid, etc). Plastic deformation occurs in collisions which create strains and stresses that exceed a certain threshold, leaving permanent changes in the shape of the grains (an example of hysteresis)[11]. Viscoelastic dissipation occurs because the relaxation of the excited internal modes occurs much faster than the time-scale for the external perturbations. The internal modes "adapt" fast to the new environment created by the external perturbation[12]. When the latter are removed, the grain's shape relaxes to the original form if the deformation does not exceed the plastic threshold.

The object of our study will be the viscoelastic mechanism of dissipation. We will base our developments on a theory developed by Schofield and Oppenheim[13], in order to obtain the transport coefficients that govern the irreversible transfer of kinetic energy to the internal degrees of freedom. The internal relaxation time-scale is shown to be fundamental to the viscoelastic dissipative mechanism[12].

1.4 Expansion and time extension techniques

Starting with the Liouville equation for the complete GS (internal and external degrees of freedom), we take advantage of the different physical time-scales of the system in order to make it tractable.

In order to do so, we need to identify and separate the degrees of freedom into fast (internal) and slow (external or kinetic) ones[14]. Averaging over the fast degrees of freedom while keeping the external ones, yields a Fokker-Planck equation that governs the behavior of the distribution for the granular (external) degrees of freedom[13].

Based on that equation, we obtain a generalized BBGKY hierarchy for the multi-grain distribution. From that hierarchy, we can obtain the kinetic equations that describe the temporal behavior of the one-body distribution. We will use techniques similar to that of Bogoliubov, in order to truncate the generalized BBGKY at some convenient point[15].

By extending the time variable into many different time-scales associated with the physical time-scales of the GS (collisional, dissipative, internal relaxation, etc.) we can isolate the correct behavior of the system on the appropriate time-scale, thus avoiding the appearance of secular terms that render the approximation invalid at longer time-scales.

1.5 Application to the rarified granular gas (GG)

Using the kinetic equations obtained above (generalized Boltzmann equations), we proceed to investigate, in more detail, the behavior of GS. Up to this point, we have studied the collision between grains, energy dissipation and the behavior of the distributions for the granular degrees of freedom. The next step will be to analyze the hydrodynamic behavior of the system. Two cases of interest present themselves: the homogeneous and the non-homogeneous GG.

The study of the homogeneous GG (a somewhat unrealistic system) permits us to understand the way kinetic energy is lost irreversibly, as a function of time[16]. The more realistic non-homogeneous model permits us to study transport properties and some of the characteristics of GS. Among those, we are specially interested in evidence for the appearance of instabilities in the homogeneous density profile that are associated with the phenomena of clustering of the grains[17].

1.6 Limitations of the model and possible extensions

The points in which the present kinetic model is somewhat limited are basically.

- Low density expansions: most applications of granular flow correspond to regimes in which the density is high.
- Small gradients: in general, GS are extremely lumpy. fluctuations of density happen on the length scale of a grain.
- Only two-body collisions are taken into account. In real systems, simultaneous collisions, in which static friction plays an important role, are the norm.

Despite the theoretical limitations presented above, kinetic models are known to work well for real and simulated systems. The breakdown occurs when the rate of collisions per particle increases quickly, during cluster formation. The multi-body collisions become non-negligeable then.

With that in mind, we will limit ourselves to the goal of finding an appropriate way to describe the low density flow phase.

Future improvements of the model might allow for

- Treatment of non-identical grains of different sizes and of non-spherical shape.
- Higher density systems, in the manner of the Enskog solution of the Boltzmann equations.
- Calculations that use higher order diagrammatic expansions of the generalized BBGKY hierarchy in order to account for simultaneous multiple collisions.

Chapter 2

A Model of Inelastic Dissipation for Granular Particles

2.1 Introduction

The term granular system designates a wide range range of physical systems that are characterized by certain common features[2]: they exist in macroscopic portions (grains), which, in the dry state, interact mainly repulsively through rigid elastic interactions; there is contact friction between the grains; and energy is dissipated during collisions due to the excitation of the internal modes. Sand, powders, particles in planetary rings[18], salt and sugar, grains in a silo[19] are just a few of the many examples of granular systems. These systems are extremely important for a number of industrial applications[20] (transport properties of powder or grains, mixtures of grains and fluids, etc). Thus, it is important to understand their flow properties [2, 21, 22]. The loss of kinetic energy via heating the grains makes the granular gas fundamentally different from a molecular system[1] and an important medium to study non-equilibrium phenomena. Granular systems present a rich variety of behavior ranging from solid-like to liquid-like, depending on the external stresses applied to the system[23].

The inelastic character of granular collisions can be summarized in terms of a coefficient of restitution which is a proportionality relation between the final and initial relative velocities in a collision. Even though the coefficient is known to depend on the initial relative velocity[24], for simplicity and computational economy, several authors have assumed it to be independent of the collision parameters[2, 21, 22]. In order to improve the understanding of instantaneous energy dissipation, some authors have tried to model relative velocity-dependent dissipation functions. Self-consistent dimensional arguments were used[20], but a more promising line assumes that the collision is slow enough so that a weak viscoelastic frictional force is superimposed onto the elastic repulsive force[9, 10].

In the present study, we propose to investigate a simple microscopic model for harmonic grains. Under the assumption that the collisions are slow enough so that no plastic deformations occur, the present model reproduces the results obtained using a viscoelastic interaction between the grains [9, 10].

This chapter is organized as follows: In section 2, we develop the model for the potential energy of deformed harmonic grains from the classical harmonic crystal model. In section 3, we study the case of two interacting grains. In section 4, a transport coefficient describing the instantaneous kinetic energy dissipation is obtained. In section 5, we obtain the equation of motion for colliding grains and evaluate the magnitude of the dissipative term. In section 6, we present a brief summary of our results.

2.2 Deformations and Potential Energy

In this section we derive the potential energy of a deformed spherical granular particle. We assume that its atoms interact through microscopic two-body potentials. The atoms in the granular particles (GP) are arranged in a crystalline lattice form. Let $\mathbf{R}_i$ denote the equilibrium, non-deformed position of atom i, ($\mathbf{R}_i \equiv a\hat{\mathbf{a}} + b\hat{\mathbf{b}} + c\hat{\mathbf{c}}$, where $\hat{\mathbf{a}}, \hat{\mathbf{b}}, \hat{\mathbf{c}}$ are the Bravais lattice basis vectors, and a, b, c are integers)[25]. Let $\boldsymbol{\rho}_i$ denote the displacement from equilibrium for atom i, and let $\mathbf{u}_i \equiv \mathbf{u}(\mathbf{R}_i)$ denote the displacement of atom i's equilibrium position due to external constraints. The atom's actual position, $\mathbf{d}_i$, is therefore given by:

$$\mathbf{d}_i = \mathbf{R}_i + \mathbf{u}_i + \boldsymbol{\rho}_i.$$

The distance between two atoms in the deformed medium is then a function of the initial undeformed distance and of the elastic and thermal displacements,

$$\mathbf{d}_{ij} = (\mathbf{R}_j - \mathbf{R}_i) + (\mathbf{u}_j - \mathbf{u}_i) + \left(\boldsymbol{\rho}_j - \boldsymbol{\rho}_i\right). \tag{2.1}$$

The difference $\mathbf{u}_j - \mathbf{u}_i$ depends on the deformation experienced by the crystal. If $\mathbf{R}_j - \mathbf{R}_i$ is small compared to the characteristic length associated with the deformations, we obtain

$$\begin{aligned} \mathbf{u}_j - \mathbf{u}_i &\approx (\mathbf{R}_j - \mathbf{R}_i) \,.\, \nabla_{\mathbf{R}} \mathbf{u}(\mathbf{R})]_{\mathbf{R}=\mathbf{R}_i} \\ &= (\mathbf{R}_j - \mathbf{R}_i)_\beta \frac{\partial}{\partial x_\beta} \mathbf{u}(\mathbf{x})\Big]_{\mathbf{x}=\mathbf{R}_i}, \end{aligned} \tag{2.2}$$

where greek subscripts denote coordinate indices and repeated indices imply summation (for $\beta = 1, 2, 3$). The distance between atoms i and j is then given by

$$\mathbf{d}_{ij} = (\mathbf{R}_j - \mathbf{R}_i) + (\mathbf{R}_j - \mathbf{R}_i)_\beta \frac{\partial}{\partial x_{i\beta}} \mathbf{u}(\mathbf{R}_i) + \left(\boldsymbol{\rho}_j - \boldsymbol{\rho}_i\right). \tag{2.3}$$

We will assume that effects associated with displacement of dislocations and other crystal defects are small. Thus, we can expand the total crystal potential energy around the new positions of the atoms up to second order in the variations of the positions. By expanding the potential

$$\Phi = \frac{1}{2} \sum_i \sum_{i \neq j} \phi_{ij}$$

around the equilibrium distance of $(\mathbf{R}_j - \mathbf{R}_i)$ [26], we obtain:

$$\phi_{ij} = \phi(\mid \mathbf{d}_{ij} \mid),$$

$$\begin{aligned}\phi_{ij} &\approx \phi(|\mathbf{R}_j-\mathbf{R}_i|)+(\boldsymbol{\beta}_{ij}.\nabla)\phi(|\mathbf{R}_j-\mathbf{R}_i|)+\\ &+\frac{1}{2}(\boldsymbol{\beta}_{ij}.\nabla)^2\phi(|\mathbf{R}_j-\mathbf{R}_i|),\\ \Phi &\approx \frac{1}{2}\sum_{i,j}\phi(|\mathbf{R}_j-\mathbf{R}_i|)+\\ &+\frac{1}{4}\sum_{i,j}(\boldsymbol{\beta}_{ij}.\nabla)^2\phi(|\mathbf{R}_j-\mathbf{R}_i|),\end{aligned}\tag{2.4}$$

up to quadratic order, where $\boldsymbol{\beta}_{ij}=\boldsymbol{\beta}_j-\boldsymbol{\beta}_i=(\mathbf{R}_j-\mathbf{R}_i).\nabla\mathbf{u}+\left(\boldsymbol{\rho}_j-\boldsymbol{\rho}_i\right)$, and the indices i and j run over all atoms in the GP.

We define the matrix $\mathbf{D}^{ij}_{\mu\nu}$:

$$\mathbf{D}^{ij}_{\mu\nu}=\delta_{i,j}\sum_k\frac{\partial^2\phi_{ik}}{\partial x_\mu\partial x_\nu}-\frac{\partial^2\phi_{ij}}{\partial x_\mu\partial x_\nu}.\tag{2.5}$$

With the properties:

$$\begin{aligned}\mathbf{D}^{ij}_{\mu\nu} &= \mathbf{D}^{ji}_{\nu\mu},\\ \mathbf{D}^{ij}_{\mu\nu} &= \mathbf{D}^{ij}_{\nu\mu},\\ \sum_i^{all\ atoms}\mathbf{D}^{ij}_{\mu\nu} &= 0.\end{aligned}$$

Thus Φ can be written in the form

$$\Phi=\frac{1}{2}\sum_{i,j}\phi(|\mathbf{R}_j-\mathbf{R}_i|)+\frac{1}{2}\sum_{i,j}\beta_{i\mu}\mathbf{D}^{ij}_{\mu\nu}\beta_{j\nu}.\tag{2.6}$$

The potential Φ can be separated into ground state energy, harmonic potential, elastic potential and coupling parts as follows:

$$\begin{aligned}\Phi &= \Phi_0+\frac{1}{2}\sum_{i,j}\rho_{i\mu}\mathbf{D}^{ij}_{\mu\nu}\rho_{j\nu}+\\ &+\frac{1}{2}\sum_{i,j}R_{i\alpha}\mathbf{D}^{ij}_{\mu\nu}R_{j\beta}\frac{\partial u_\mu}{\partial x_\alpha}\frac{\partial u_\nu}{\partial x_\beta}+\\ &+\sum_{i,j}R_{i\alpha}\mathbf{D}^{ij}_{\mu\nu}\frac{\partial u_\mu}{\partial x_\alpha}\rho_{j\nu},\end{aligned}\tag{2.7}$$

where $\Phi_0 = \sum_j \sum_{i<j} \phi(|\mathbf{R}_j - \mathbf{R}_i|)$.

The elastic potential term (due to the deformation) which is given by

$$V_{el} = \frac{1}{2} \sum_{i,j} R_{i\alpha} \mathbf{D}^{ij}_{\mu\nu} R_{j\beta} \frac{\partial u_\mu}{\partial x_\alpha}(\mathbf{R}_i) \frac{\partial u_\nu}{\partial x_\beta}(\mathbf{R}_j),$$

accounts for the classical elastic energy of the material [25]. Using the properties of $\mathbf{D}^{ij}_{\mu\nu}$ we can rewrite V_{el} in the form:

$$V_{el} = \frac{1}{2} \sum_{j} E_{\alpha\mu\beta\nu} \frac{\partial u_\mu}{\partial x_\alpha}(\mathbf{R}_j) \frac{\partial u_\nu}{\partial x_\beta}(\mathbf{R}_j),$$

where the derivatives of $\mathbf{u}$ are taken at the point $\mathbf{R}_i$ and

$$E_{\alpha\mu\beta\nu} = -\frac{1}{2} \sum_{i}^{allatoms} R_{i\alpha} \mathbf{D}_{\mu\nu}(\mathbf{R}_i) R_{i\beta}.$$

The above expression can be further transformed by noticing that a pure rotation does not change the solid energy. This implies that V_{el} can depend on $\frac{\partial u_\nu}{\partial x_\beta}$ only through the strain tensor, which for small deformations has the form

$$u_{\alpha\beta} = \frac{1}{2} \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right). \tag{2.8}$$

The elastic term then becomes[25]

$$V_{el} = \frac{1}{2} \sum_{j} E_{(\alpha\mu)(\beta\nu)} u_{\alpha\mu}(\mathbf{R}_j) u_{\nu\beta}(\mathbf{R}_j), \tag{2.9}$$

where the symbols $(\alpha\mu)$ and $(\beta\nu)$ denote the symmetric part of $E_{(\alpha\mu)(\beta\nu)}$ with respect to $(\alpha\mu)$ and $(\beta\nu)$ respectively.

The term

$$V_\phi = \sum_{i,j} R_{i\alpha} \mathbf{D}^{ij}_{\mu\nu} \frac{\partial u_\mu}{\partial x_\alpha}(\mathbf{R}_i) \rho_{j\nu},$$

is responsible for the coupling between the internal degrees of freedom, $\boldsymbol{\rho}_i$, and the distance between the two GPs centers of mass, through the derivative $\frac{\partial u_\mu}{\partial x_\alpha}$, which can be taken at $\mathbf{R}_j$ to a very good approximation.

Due to a similar argument to (2.9), we can write the coupling term as

$$V_\phi = \sum_j E_{(\alpha\mu)\nu} u_{\alpha\mu} \rho_{j\nu}, \tag{2.10}$$

where $E_{(\alpha\mu)\nu}$ is the symmetric tensor (on $\alpha\mu$) given by

$$E_{(\alpha\mu)\nu} = -\frac{1}{4} \sum_j \left(R_{j\alpha} \mathbf{D}_{\mu\nu}(\mathbf{R}_j) + R_{j\mu} \mathbf{D}_{\alpha\nu}(\mathbf{R}_j) \right). \tag{2.11}$$

2.3 Interaction Between Two Granular Particles

When two GPs interact, the results of section 2 must be generalized to include cross-terms between the degrees of freedom of the two grains. We have to take into account the terms that correspond to direct interaction between GPs 1 and 2. Before doing the expansion for ϕ_{ij} (where i belongs to particle 1 and j belongs to particle 2), we can eliminate those ϕ_{ij}'s which are small (those for which $\mid \mathbf{r}_{ij} \mid \gg r_0 \equiv$ interaction range of the order of the lattice parameter). Since this is a short range interaction, only those atoms close to the interface between particles 1 and 2 will contribute. Their number being proportional to the area of the interface, we will neglect them in comparison with the bulk contribution to the coupling energy. The coupling potential can then be written as (where the superscripts denote the grain)

$$V_\phi = \sum_j^{(1)} E^{(1)}_{(\alpha\mu)\nu} u^{(1)}_{\alpha\mu} \rho^{(1)}_{j\nu} + \sum_j^{(2)} E^{(2)}_{(\alpha\mu)\nu} u^{(2)}_{\alpha\mu} \rho^{(2)}_{j\nu}. \tag{2.12}$$

where the superscripts (1) and (2) denote particles 1 and 2, and the strain tensor depends on the Bravais summation index. We are going to use the convention that whenever there is a sum over Bravais vectors on the following, the strain tensor depends on the summation index.

The total elastic contribution will be

$$V_{el} = \frac{1}{2} \sum_i^{(1)} E^{(1)}_{(\alpha\mu)(\beta\nu)} u^{(1)}_{\alpha\mu} u^{(1)}_{\nu\beta} + \frac{1}{2} \sum_i^{(2)} E^{(2)}_{(\alpha\mu)(\beta\nu)} u^{(2)}_{\alpha\mu} u^{(2)}_{\nu\beta}, \tag{2.13}$$

and the total harmonic contribution is given by

$$\begin{aligned} V_H &= \frac{1}{2}\sum_{i,j}^{(1)}(\rho^{(1)}_{j\mu} - \rho^{(1)}_{i\mu})\mathbf{D}^{(1)ij}_{\mu\nu}(\rho^{(1)}_{j\nu} - \rho^{(1)}_{i\nu}) + \\ &+\frac{1}{2}\sum_{i,j}^{(2)}(\rho^{(2)}_{j\mu} - \rho^{(2)}_{i\mu})\mathbf{D}^{(2)ij}_{\mu\nu}(\rho^{(2)}_{j\nu} - \rho^{(2)}_{i\nu}). \end{aligned} \tag{2.14}$$

2.4 Dissipation of Energy

Schofield and Oppenheim[13] proposed a mechanism for the dissipation of energy that occurs when two GP (1 and 2) collide. It is mediated by a transport coefficient defined as follows:

$$\gamma(r_{12}) = \int_0^\infty d\tau < \nabla\hat{V}_\phi e^{-L_{in}\tau}\nabla\hat{V}_\phi >_f, \tag{2.15}$$

where $< ... >_f$ means a statistical average keeping the center of masses fixed, L_{in} is the Liouvillian operator for the internal granular degrees of freedom only, (i.e., center of mass positions and total momentum are kept fixed), and $\hat{A} = A- < A >_f$. The typical variation of $\mid \boldsymbol{\rho}_i \mid$ is smaller than a, the typical lattice spacing. Given that the typical macroscopic deformation is h, and σ is the GP's diameter, we have the inequalities $a \ll h \ll \sigma$.

The coefficient $\gamma(r_{12})$ will be given to lowest order in the strain tensor (which is assumed to be small) by[13]

$$\gamma(r_{12}) = \int_0^\infty d\tau < \nabla\hat{V}_\phi e^{-L_{harm}\tau}\nabla\hat{V}_\phi >_f .$$

The linearity of V_ϕ in $\boldsymbol{\rho}_i$ leads to $\nabla\hat{V}_\phi = \nabla V_\phi$, due to the symmetry of a harmonic oscillator. Cross averages like $< \boldsymbol{\rho}^{(1)}_j \boldsymbol{\rho}^{(2)}_k >_f$ will also vanish. Thus, we have for $\gamma(r_{12})$

$$\begin{aligned} \gamma(r_{12}) &= \sum_{i,j}^{(1)} E^{(1)}_{(\alpha\mu)\nu}E^{(1)}_{(\beta\gamma)\theta}(\nabla_{12}u^{(1)}_{\beta\gamma})(\nabla_{12}u^{(1)}_{\alpha\mu}) \times \\ &\int_0^\infty d\tau < \rho^{(1)}_{i\nu}\rho^{(1)}_{j\theta}(\tau) >_f + \\ &+\sum_{i,j}^{(2)} E^{(2)}_{(\alpha\mu)\nu}E^{(2)}_{(\beta\gamma)\theta}(\nabla_{12}u^{(2)}_{\beta\gamma})(\nabla_{12}u^{(2)}_{\alpha\mu}) \times \end{aligned}$$

$$\int_0^\infty d\tau < \rho^{(2)}_{i\nu}\rho^{(2)}_{j\theta}(\tau) >_f, \tag{2.16}$$

where $\nabla_{12} = \nabla_{\mathbf{r}_{12}}$.

The harmonic form for the potential gives in first approximation[14, 2

$$< \rho_{i\nu}\rho_{j\theta}(\tau) >_f = \mathbf{D}^{-1ij}_{\nu\theta} k_B T F(\tau), \tag{2.17}$$

where the correlation function $F(\tau)$ can be assumed to decay fast for a large range of interatomic potentials to insure the convergence of the time integrals. We will assume the form[27]

$$F(\tau) = e^{-\tau/\tau_v},$$

where τ_v sets the vibrational time scale. The time integrals in equation(2.16) become $\tau_v \mathbf{D}^{-1ij}_{\nu\theta} kT$.

Since the particles are identical, we can re write $\gamma(r_{12})$ as

$$\begin{aligned} &\gamma(r_{12}) \\ &= \tau_v \sum_{i,j} E_{(\alpha\mu)\nu} E_{(\beta\gamma)\theta} \mathbf{D}^{-1ij}_{\nu\theta} \times \\ &\quad \left((\nabla_{12} u^{(1)}_{\beta\gamma})(\nabla_{12} u^{(1)}_{\alpha\mu}) + (\nabla_{12} u^{(2)}_{\beta\gamma})(\nabla_{12} u^{(2)}_{\alpha\mu}) \right). \end{aligned} \tag{2.18}$$

Equation (2.18) describes the energy dissipation occurring during the collision of two GPs, as will be seen in the next section.

2.5 Dissipative Equation of Motion

When two identical GPs of mass m collide, kinetic energy is dissipated through excitation of the internal modes of vibration. In our simple model we neglect plastic deformation effects. Since the collision time is much longer than the vibrational time ($\tau_c \gg \tau_v$), we can assume that the interaction between two GPs is very well described by the elastic Hertzian quasi-static force[28]. The form for the interparticle interaction can also be obtained from a Fokker-Planck equation for the probability distribution $W(X_t, t)$ of a granular system[13]:

$$\begin{aligned} &\dot{W}(X_t, t) \\ &= \Bigg[\Bigg(-\sum_{i=1}^{N} \frac{\mathbf{p}_i}{m}.\nabla_{r_i} + \sum_{i=1}^{N} \nabla_{r_i}(U+\omega).\nabla_{\mathbf{p}_i}\Bigg) + \\ &+\frac{1}{2}\sum_{j}^{N}\sum_{k\neq j}^{N} \gamma_{jk}\hat{\mathbf{r}}_{jk}\hat{\mathbf{r}}_{jk} : (\nabla_{\mathbf{p}_j} - \nabla_{\mathbf{p}_k}) \\ &\Bigg((\nabla_{\mathbf{p}_j} - \nabla_{\mathbf{p}_k}) + \beta\frac{\mathbf{p}_j - \mathbf{p}_k}{m}\Bigg)\Bigg] W(t), \end{aligned} \tag{2.19}$$

where $\mathbf{p}_i, \mathbf{r}_i, i = 1, ..., N$ are the momenta and positions, respectively, of the centers of mass of the grains, $X_t = \{\mathbf{p}^N, \mathbf{r}^N\}$, $\beta = \frac{1}{k_B T}$, where T is the internal temperature of the GPs, $\gamma_{jk} = \gamma(r_{jk})$ is the dissipative coefficient calculated in section 4 and $\hat{\mathbf{r}}_{jk}$ is the unit vector in the direction between particles j and k, and $U + \omega$ is the effective interaction potential between the grains.

In the case of two particles, we define $\mathbf{r}_{1,2}(t) =< \mathbf{r}_{1,2} >_t$ and $\mathbf{v}_{1,2}(t) =< \dot{\mathbf{r}}_{1,2} >_t$, where $< B >_t= \int dX_t W(t) B$. Assuming that $W(X_t, t)$ is sharply peaked, we can approximate $\mathbf{v}_{1,2}(t) \approx \dot{\mathbf{r}}_{1,2}(t)$. We also define relative and center of mass coordinates:

$$\begin{aligned} \mathbf{r}_{12} &= \mathbf{r}_2 - \mathbf{r}_1, \\ \mathbf{r}_{cm12} &= \frac{1}{2}(\mathbf{r}_2 + \mathbf{r}_1). \end{aligned}$$

The deformation parameter h is defined as

$$h = \begin{cases} \sigma - r_{12} & \text{if } \sigma \geq r_{12} \\ 0 & \text{otherwise} \end{cases},$$

where σ is the diameter of a GP.

From the basic result

$$\frac{d}{dt} < B >_t= \int dX_T \dot{W} B,$$

and equation(19), after assuming that $U + \omega \approx V_{12}^{el}$, we obtain

$$\begin{aligned}
&< \dot{\mathbf{p}}_2 >_t - < \dot{\mathbf{p}}_1 >_t \\
= &\int dX_t(\mathbf{p}_2 - \mathbf{p}_1)\left(\nabla_{\mathbf{r}_1} V_{12}^{el}.\nabla_{\mathbf{p}_1} + \nabla_{\mathbf{r}_2} V_{12}^{el} \nabla_{\mathbf{p}_2}\right) W(t) + \\
&+ \int dX_t \gamma_{12} \hat{\mathbf{r}}_{12} (\mathbf{p}_2 - \mathbf{p}_1) \hat{\mathbf{r}}_{12} : \\
&: (\nabla_{\mathbf{p}_1} - \nabla_{\mathbf{p}_2}) \left((\nabla_{\mathbf{p}_1} - \nabla_{\mathbf{p}_2}) + \beta \frac{\mathbf{p}_1 - \mathbf{p}_2}{m}\right) W(t), \\
= &- \int dX_t W(t) \left(\nabla_{\mathbf{r}_2} V_{12}^{el} - \nabla_{\mathbf{r}_1} V_{12}^{el}\right) - \\
&- \beta \int dX_t \gamma_{12} \hat{\mathbf{r}}_{12} \hat{\mathbf{r}}_{12}. \frac{\mathbf{p}_1 - \mathbf{p}_2}{m} W(t), \\
= &< \mathbf{F}_{12}^{el} >_t - \frac{\beta}{m} < \gamma_{12} \hat{\mathbf{r}}_{12} \hat{\mathbf{r}}_{12}.(\mathbf{p}_1 - \mathbf{p}_2) >_t,
\end{aligned}$$

where $\mathbf{F}_{12}^{el} = -V_{12}^{el}(h)' \hat{\mathbf{r}}_{12}$.

The elastic potential between the grains is a function of the tensor $E_{(\alpha\mu)(\beta\gamma)}$ defined in equation (2.9). The microscopic summation form of V_{12}^{el} reduces to the usual macroscopic elastic energy derived from phenomenological theories. In terms of the particles Young modulus E, Poisson ratio Σ, and radius $\frac{\sigma}{2}$, $V_{12}^{el}(h)$ in equation(2.13) can be derived, and is given by[9, 29]

$$V_{12}^{el}(h) = \frac{1}{2} k h^{\frac{5}{2}}, \tag{2.20}$$

where for three-dimensional isotropic spheres[28]

$$k = \left(\frac{8}{15\sqrt{2}}\right) \frac{E}{1 - \Sigma^2} R^{\frac{1}{2}}.$$

The equation for the time variation of h for a frontal collision becomes

$$\frac{m}{2} \frac{d^2 h}{dt^2} = -\frac{5}{4} k h^{\frac{3}{2}} - \frac{\beta \gamma(h)}{m} \frac{dh}{dt}. \tag{2.21}$$

In the equation above, we observe that the energy dissipation is described by a frictional force mediated by $\gamma(r_{12})$

$$\mathbf{F}_f = -\frac{\beta\gamma(r_{12})}{m}(\hat{\mathbf{k}}.\mathbf{p}_{12})\hat{\mathbf{k}}.$$

We will next evaluate $\gamma(r_{12}) \equiv \gamma(h)$ as a function of h so that way we can solve equation (2.21) and thus determine the velocity dependent coefficient of restitution for a quasi-elastic collision.

2.6 The Frictional Coefficient γ

From equation (2.18), the expression for $\gamma(h)$ when the particles are identical is given by

$$\begin{aligned} \gamma(h) &= \sum_j F_{(\alpha\mu)(\beta\gamma)} \Big((\nabla_{12} u^{(1)}_{\beta\gamma})(\nabla_{12} u^{(1)}_{\alpha\mu}) + \\ &\quad + (\nabla_{12} u^{(2)}_{\beta\gamma})(\nabla_{12} u^{(2)}_{\alpha\mu}) \Big), \qquad (2.22) \end{aligned}$$

where $F_{(\alpha\mu)(\beta\gamma)} = \tau_v kT E_{(\alpha\mu)\nu} E_{(\beta\gamma)\theta} \mathbf{D}^{-1ij}_{\nu\theta}$.

The behavior of $\gamma(h)$ can be obtained by a scaling argument following Landau[28]. The equation for the radius of the contact region, b, as a function of the curvature of the particle, $A = \frac{2}{\sigma}$, where σ is the diameter of the particles, is given by[28]

$$A = \frac{FD}{\pi}\int_0^\infty \frac{d\xi}{(b^2+\xi)^2(\xi)^{\frac{1}{2}}}.$$

The deformation h is given by[28]

$$h = \frac{FD}{\pi}\int_0^\infty \frac{d\xi}{(b^2+\xi)(\xi)^{\frac{1}{2}}},$$

where F is the force between the spheres and[28]

$$D = \frac{3}{2}\left(\frac{1-\Sigma^2}{E}\right).$$

In order to keep the above equations invariant, we scale lengths by a factor $\sqrt{\alpha}$ ($b \to \sqrt{\alpha} b$, $\xi \to \alpha\xi$ and $\mathbf{x} \to \sqrt{\alpha}\mathbf{x}$), and the force by a factor $\alpha^{\frac{3}{2}}$ ($F \to \alpha^{\frac{3}{2}} F$). We then obtain for $h \to \alpha h$, showing that the force varies as $h^{\frac{3}{2}}$[29]. The z-component (collision axis) for the deformation vector $u_z(\mathbf{x})$ is given by[30]

$$\begin{aligned} u_z(\mathbf{x}) &= \frac{3F}{2\pi a^2} \int_{x'^2+y'^2 \leq b^2} \frac{dx'dy'}{\sqrt{(x-x')^2+(y-y')^2+z^2}} \times \\ &\quad \times \sqrt{1-\frac{x'^2+y'^2}{b^2}}. \end{aligned} \tag{2.23}$$

Using the variable $\mathbf{x}'' = b\mathbf{x}'$, we show that $u_z(\mathbf{x})$ scales as

$$u_z(\mathbf{x}) \to u_z(\sqrt{\alpha}\mathbf{x}) = \alpha u_z(\mathbf{x}). \tag{2.24}$$

From above, we obtain the scaling behavior of the strain tensor:

$$u_{\alpha\beta}(\mathbf{x}) \to u_{\alpha\beta}(\sqrt{\alpha}\mathbf{x}) = \sqrt{\alpha} u_{\alpha\beta}(\mathbf{x}). \tag{2.25}$$

The tensors $E_{(\alpha\mu)(\beta\gamma)}$ and $F_{(\alpha\mu)(\beta\gamma)}$ are invariant under the α scale transformation. The derivatives of the strain tensor scale as

$$\frac{\partial u_{\alpha\beta}(\mathbf{x})}{\partial h} \to \frac{\partial u_{\alpha\beta}(\sqrt{\alpha}\mathbf{x})}{\alpha \partial h} = \frac{1}{\sqrt{\alpha}} \frac{\partial u_{\alpha\beta}(\mathbf{x})}{\partial h}. \tag{2.26}$$

We deduce from this that the total elastic energy scales as $\alpha^{\frac{5}{2}}$ and the dissipative function $\gamma(h)$ as $\alpha^{\frac{1}{2}}$, implying that $V_{el} \propto h^{\frac{5}{2}}$ and $\gamma(h) \propto h^{\frac{1}{2}}$.

Due to the scaling properties of the strain tensor $u_{\alpha\beta}$ and its derivative $\frac{\partial u_{\alpha\beta}(\mathbf{x})}{\partial h}$, we can write

$$\frac{\partial u_{\alpha\beta}(\mathbf{x})}{\partial h} = \frac{B}{h} u_{\alpha\beta}(\mathbf{x}),$$

where B is a proportionality constant.

We deduce from the above and equation (2.22) that

$$\gamma(h) = \sum_j \mathcal{F}_{(\alpha\mu)(\beta\gamma)} \left(u^1_{\beta\gamma} u^1_{\alpha\mu} + u^2_{\beta\gamma} u^2_{\alpha\mu} \right) h^{-2}, \tag{2.27}$$

where $\mathcal{F}_{(\alpha\mu)(\beta\gamma)} = B^2 F_{(\alpha\mu)(\beta\gamma)}$. The tensor $\mathcal{F}_{(\alpha\mu)(\beta\gamma)}$ possesses the same symmetry properties as $E_{(\alpha\mu)(\beta\gamma)}$. Consequently, $\gamma(h)$ will be a function of different phenomenological parameters but of the same form as $V_{el} \equiv V_{el}(E, \Sigma)$.

Given that the elastic force between the GP is obtained by taking the derivative of V_{el} equation (2.20) with respect to h, we obtain for $\gamma(h)$ in equation (2.22)

$$\gamma(h) = \frac{5}{2} k' h^{\frac{5}{2}} h^{-2} = \frac{5}{2} k' h^{\frac{1}{2}}, \tag{2.28}$$

where k' is a function of the tensor $\mathcal{F}_{(\alpha\mu)(\beta\gamma)}$, and has the same form as k with $E \to \eta_1$ and $\Sigma \to \eta_2$, where η_1 and η_2 are the corresponding viscoelastic coefficients.

The equation of motion for the GP on a frontal collision then becomes

$$\frac{m}{2} \frac{d^2 h}{dt^2} = \frac{5}{4} k h^{\frac{3}{2}} - \frac{5}{2} k' h^{\frac{1}{2}} \frac{dh}{dt}. \tag{2.29}$$

Equation (2.29) reproduces results obtained by heuristic methods[9, 10].

The above equation will describe the behavior of smooth spherical GP at speeds much smaller than the speed of sound inside the grain.

The relative importance of dissipation can be obtained by assuming typical values for the physical parameters in question. The typical interatomic potential is denoted by ϕ_0, the typical value of $u_{\alpha\beta}$ is u, the typical elastic energy is $\phi \approx \sum \phi_0 u u$, the typical lattice spacing is a. We may assume $\phi \approx kT_g$ (hard-sphere approximation), where T_g is the granular temperature, and $mv_g^2 \approx kT_g$.

The coupling tensors are given by

$$\mathbf{D}_{\mu\nu} \approx \frac{\phi_0}{a^2}, \ \mathbf{E}_{(\mu\nu)(\alpha\beta)} \approx \phi_0,$$

thus showing why $\phi \approx \sum \phi_0 u u$. In addition, we obtain for the symmetric tensor

$\mathbf{E}_{(\mu\nu)\alpha}$

$$\mathbf{E}_{(\mu\nu)\alpha} \approx \frac{\phi_0}{a},$$

and the typical correlation function

$$\int d\tau < xx(t) > \approx \frac{kTa^2\tau_v}{\phi_0}.$$

Thus, we obtain for γ

$$\gamma \approx \sum \frac{\phi_0^2}{a^2}\frac{u^2}{L^2}\frac{kTa^2\tau_v}{\phi_0} \approx \frac{kT\tau_v}{L^2}\sum \phi_0 uu \approx \frac{kT\tau_v\phi}{L^2},$$

where L corresponds to the typical deformation length with $L \ll \sigma$.

We are now prepared to evaluate the inelastic term in the fundamental Fokker-Planck equation for the distribution, $W \equiv W(\mathbf{r}^N, \mathbf{p}^N)$, which is a function of the granular degrees of freedom $\{\mathbf{r}^N, \mathbf{p}^N\}$. Let τ be an arbitrary time-scale, and let the terms with asterisks be dimensionless $(O(1))$. Given that O^* is a second order differential operator, the dissipative contribution will be[13]

$$\frac{1}{\tau}\frac{\partial W}{\partial t^*} \approx \frac{\gamma}{m^2 v_g^2}\frac{kT_g}{kT}O^*W.$$

Replacing the value obtained for γ, we have

$$\frac{1}{\tau}\frac{\partial W}{\partial t^*} \approx \frac{kT\tau_v\phi}{L^2}\frac{1}{m^2v_g^2}\frac{kT_g}{kT}O^*W \approx \frac{\phi\tau_v}{mL^2}O^*W.$$

Letting $\tau_i \approx \frac{L}{v_g}$, where τ_i is the time a granular particle takes to move a distance corresponding to its deformation length ($\sim L$), we obtain

$$\frac{1}{\tau}\frac{\partial W}{\partial t^*} \approx \frac{\tau_v}{\tau_i^2}O^*W.$$

If we set the time-scale $\tau = \tau_i$, we obtain

$$\frac{\partial W}{\partial t^*} \approx \left(\frac{\tau_v}{\tau_i}\right)O^*W. \quad (2.30)$$

So we observe that the order of magnitude of the dissipative term on the time-scale of τ_i with respect to the streaming term is given roughly by the ratio between the granular velocity and the velocity of sound in the material that constitute the grains. The relative order of magnitude of the dissipative term in the Fokker-Planck equation for W relative to the streaming term is given approximatively by

$$\frac{\tau_v \tau_c}{\tau_i^2} \approx \frac{\sigma}{L} \frac{v_g}{v_s}.$$

For typical $v_{sound} \sim 10^3 - 10^4 v_g$ and $\frac{L}{\sigma} \sim 10^{-2}$, one sees that the ratio is small as expected, but not extremely small.

In a recent paper [10], the authors propose a model which implies that in order to break the asperities of the surface of two grains (plastic deformation) in contact, the tangential stress (which is a function of shear deformation) has to exceed a material dependent threshold. In other words, the collision has to be energetic enough to conquer the elastic potential barrier. We believe then, that the present viscoelastic frictional model will describe satisfactorily slow collisions for rough and also smooth granular systems (in which case the energy dissipated by plastic deformations of asperities will be far smaller than that for typical systems found in nature).

2.7 Discussion

We obtain the coefficient of instantaneous energy dissipation for collisions between two grains by an appropriate separation of the potential energy into internal, granular and coupling parts and with the help of a first principles theory for granular distribution functions.

The form for the dissipative coefficient $\gamma(r)$ that we obtain is identical to the ones obtained elsewhere[9, 10] assuming phenomenological viscoelastic dissipative coefficients. The agreement suggests that the phenomenological model is a plausible one to describe the interaction between GPs that do not involve plastic deformation of the grains.

We are extending the present model in order to include the case of rough granular systems.

Chapter 3

Expansion Techniques and Kinetic Theory Methods

3.1 Introduction

Put in a simple way, classical granular systems are collections of grains, formed by large numbers of atoms. One immediate consequence of that fact is the existence of two (or more) distinct time-scales that govern the system's time evolution.

One of them (τ_i) is associated with the rapid internal vibrational phenomena that involves the grains internal coordinates (positions and velocities of the atoms themselves, under the constraint that total internal momentum is zero identically).

The other (τ_g, and possibly others) is associated with the motion of the grains as a unit. It deals with the positions and velocities of the centers of mass of the grains.

The second time-scale is sufficiently slower than the first one, under usual circumstances, so that we can look for a treatment of the equations of motion that takes advantage of the small expansion parameter $\frac{\tau_i}{\tau_g}$.

The method we are going to follow consists of eliminating the fast degrees of freedom (the internal ones)[31] through an averaging of the Liouville equation for the complete system (internal + external degrees of freedom), thus obtaining a Fokker-Planck equation that describes the behavior of the external degrees of freedom. We then obtain a generalized BBGKY hierarchy for the distributions of the external degrees of freedom. By using the small parameter defined above to expand the distributions of the hierarchy, we extract the equations that describe the kinetic behavior of the system.

3.2 The basic Fokker-Planck equation

We start by outlining the method used, by Schofield and Oppenheim[13], to obtain a Fokker-Planck equation that describes the time evolution of the granular (external) degrees of freedom.

The system consists of N granular particles with translational degrees of freedom $X_t = (\mathbf{r}^N, \mathbf{p}^N)$ (mass m) and internal degrees of freedom $X_i = (\xi^N, \pi^N)$ (mass $\mu \ll m$). The Hamiltonian for the system is given by:

$$H(X_t, X_i) = H_t(X_t) + H_i(X_i) + \phi(X_t, X_i), \tag{3.1}$$

where

$$\begin{aligned} H_t(X_t) &= \frac{\mathbf{p}^N.\mathbf{p}^N}{2m} + U(\mathbf{r}^N), \\ H_i(X_i) &= \sum_{j=1}^{N} \left(\frac{\pi_j.\pi_j}{2\mu} + V(\xi_j) \right), \\ \phi(X_t, X_i) &= \sum_{i=1}^{N} \sum_{j>i} \phi(r_{ij}, \xi_i, \xi_j), \end{aligned}$$

where ξ_j(and π_j) denote all the internal coordinates (momenta) of particle j.

The potential $U(\mathbf{r}^N)$ includes the effects of external fields (e.g. gravitation) and the Hertzian interaction amongst the granular particles. Thus $U(\mathbf{r}^N)$ can be written

$$\begin{aligned} U(\mathbf{r}^N) &= U_{ext} + U_{int}, \\ &= \sum_{i=1}^{N} \tilde{u}(\mathbf{r}_i) + \sum_{i<j} u(r_{ij}). \end{aligned}$$

The potentials u_{ij} and ϕ_{ij} are short range.

The Liouvillian operator for the system is given by:

$$L = L_t + L_i + L_\phi, \tag{3.2}$$

where

$$\begin{aligned} L_t &= -\frac{\mathbf{p}^N}{m}.\nabla_{\mathbf{r}^N} + \nabla_{\mathbf{r}^N} U(\mathbf{r}^N).\nabla_{\mathbf{p}^N}, \\ L_i &= -\frac{\pi^N}{\mu}.\nabla_{\xi^N} + \nabla_{\xi^N} V(\xi^N).\nabla_{\pi^N}, \\ L_\phi &= \nabla_{\mathbf{r}^N}\phi.\nabla_{\mathbf{p}^N} + \nabla_{\xi^N}\phi.\nabla_{\pi^N}. \end{aligned}$$

By using projection operator techniques we can derive a Fokker-Planck equation for the translational degrees of freedom X_t since they change on a much slower time scale than the internal degrees of freedom.

Let the distribution for the complete system be $\rho(X_i, X_t, t)$. The Liouville equation is

$$\frac{\partial}{\partial t}\rho(X_i, X_t, t) = L\rho(X_i, X_t, t) = (L_t + L_i + L_\phi)\,\rho(X_i, X_t, t). \tag{3.3}$$

The projector operator, $\mathcal{P}$, we are going to use, to eliminate the fast degrees of freedom of the system, is defined by

$$\mathcal{P}B(X_i, X_t, t) = \tilde{\rho}(X_i, X_t, t)\int dX_i B(X_i, X_t, t), \tag{3.4}$$

where $B(X_i\ X_t, t)$ is an arbitrary dynamical function of (X_i, X_t), and $\tilde{\rho}^N(X_i, X_t, t)$ is defined in what follows.

Let $W(X_t, t) = \int dX_i\rho(X_i, X_t, t)$ be the distribution function for the translational degrees of freedom.

The equilibrium distribution is given by

$$\rho_e = \frac{e^{-\beta H}}{\int dX_i dX_t e^{-\beta H}} = \frac{e^{-\beta H}}{Z} \tag{3.5}$$

and

$$W_e = \int dX_t \rho_e = \frac{e^{-\beta H_t}}{Z} \int dX_i e^{-\beta H_i - \beta\phi}. \tag{3.6}$$

We now define

$$\tilde{\rho} = \frac{\rho_e}{W_e} = \rho_i e^{-\beta(V-\omega)},$$

where $\rho_i = \frac{e^{-\beta H_i}}{\int dX_i e^{-\beta H_i}}$ (which is the distribution for the internal degrees of freedom, irrespective of the external ones), and $\omega = -\frac{1}{\beta} \ln \int dX_i \rho_i e^{-\beta V}$, the potential of mean force.

We observe that

$$\int dX_i \frac{\partial}{\partial t} \rho = \frac{\partial}{\partial t} W,$$

and by defining $\rho = y + z$, where $y = \mathcal{P}\rho = \tilde{\rho} W$ and $z = \mathcal{Q}\rho = (1 - \mathcal{P})\rho$, we obtain

$$\dot{W} = L_t W + \sum_j^{allparticles} \int dX_i \tilde{\rho} \frac{\partial \phi}{\partial \mathbf{r}_j} . \frac{\partial}{\partial \mathbf{p}_j} W + \sum_j^{allparticles} \int dX_i \frac{\partial \phi}{\partial \mathbf{r}_j} . \frac{\partial}{\partial \mathbf{p}_j} z(t). \tag{3.7}$$

The formal solution for $z(t)$ is given by

$$z(t) = e^{QLt} z(0) + \int_0^t d\tau e^{QL\tau} L \tilde{\rho} W(t - \tau). \tag{3.8}$$

After some manipulations with equation (3.7), we have

$$\begin{aligned} \dot{W}(X_t, t) &= \left[\left(-\frac{\mathbf{p}^N}{m} . \nabla_{r^N} + \nabla_{r^N} (U + \omega) . \nabla_{\mathbf{p}^N} \right) \right. \\ &\quad \left. + \Gamma(\mathbf{r}^N) : \nabla_{\mathbf{p}^N} \left(\nabla_{\mathbf{p}^N} + \beta \frac{\mathbf{p}^N}{m} \right) \right] W(t), \end{aligned} \tag{3.9}$$

where

$$\Gamma(\mathbf{r}^N) = \int_0^\infty d\tau \int dX_i \tilde{\rho} (\nabla_{r^N} \phi) e^{(L_i + \nabla_{\xi^N} \phi . \nabla_{\pi^N})\tau} (\nabla_{r^N} \phi),$$

$\tilde{\rho}(X_i, X_t, t)$ is the conditional distribution function of the internal degrees of freedom in the presence of fixed particles[13],

$$e^{-\beta\omega} = \frac{\int dX_i \; e^{-\beta H_i - \beta\phi}}{\int dX_i \; e^{-\beta H_i}}, \tag{3.10}$$

the correlation function in $\Gamma(\mathbf{r}^N)$ decays to zero rapidly and $\beta = \frac{1}{k_B T}$ where T is the temperature of the internal degrees of freedom which is assumed to be constant in time. The potential of mean force ω can be written as a sum of two-body terms at low densities, i.e.

$$\omega(\mathbf{r}^N) = \sum_{i<j} \omega(r_{ij}).$$

Due to the short-range nature of ϕ, we can write at low densities

$$\begin{aligned} &\Gamma(\mathbf{r}^N) : \nabla_{\mathbf{p}^N}\left(\nabla_{\mathbf{p}^N} + \beta\frac{\mathbf{p}^N}{m}\right) \approx \\ &\sum_{j<k} \gamma_{jk}\hat{\mathbf{r}}_{jk}\hat{\mathbf{r}}_{jk} : (\nabla_{\mathbf{p}_j} - \nabla_{\mathbf{p}_k}) \\ &\times \left((\nabla_{\mathbf{p}_j} - \nabla_{\mathbf{p}_k}) + \beta\frac{\mathbf{p}_j - \mathbf{p}_k}{m}\right), \end{aligned} \tag{3.11}$$

where

$$\gamma_{jk} = \int_0^\infty d\tau \int dX_i \tilde{\rho}(\nabla_{r_{jk}}\phi_{jk}) e^{(L_i + \nabla_{\xi^N}\phi . \nabla_{\pi^N})\tau} (\nabla_{r_{jk}}\phi_{jk}).$$

We write then

$$\begin{aligned} &\dot{W}(X_t, t) \\ &= \Bigg[\left(-\sum_{i=1}^{N} \frac{\mathbf{p}_i}{m} . \nabla_{r_i} + \sum_{i=1}^{N}\left(\sum_{j\neq i}^{N} \mathbf{F}_{ij} + \mathbf{X}_i\right) . \nabla_{\mathbf{p}_i}\right) + \\ &\frac{1}{2}\sum_{j}^{N}\sum_{j\neq k}^{N} \gamma_{jk}\hat{\mathbf{r}}_{jk}\hat{\mathbf{r}}_{jk} : (\nabla_{\mathbf{p}_j} - \nabla_{\mathbf{p}_k}) \times \\ &\left((\nabla_{\mathbf{p}_j} - \nabla_{\mathbf{p}_k}) + \beta\frac{\mathbf{p}_j - \mathbf{p}_k}{m}\right)\Bigg] W, \end{aligned} \tag{3.12}$$

We will express the equation above in a system of units natural to the granular system under investigation. that will reduce equation (3.12) to a dimensionless form.

Our choice will be: r_0, the particle's radius for the unit of length; $\tau_i = \frac{r_0}{v_g}$, where

v_g is the typical granular velocity, for the unit of time; and the mass of a grain, m, as the unit of mass.

We can now represent the important physical quantities as a product of units and dimensionless functions (with asterisks):

$$\mathbf{p}_j = \frac{mr_0}{\tau_i}\mathbf{p}_j^*, \mathbf{F}_{ij} = \frac{mr_0}{\tau_i^2}\mathbf{F}_{ij}^*, \phi_{ij} = \frac{mr_0^2}{\tau_i^2}\phi_{ij}^*,$$

and

$$\gamma_{ij} = \frac{m^2r_0^2}{\tau_i^3}\gamma_{ij}^*, k_BT = \frac{mr_0^2}{\tau_i^2}T^*, k_BT_g = \frac{mr_0^2}{\tau_i^2}T_g^*,$$

where ϕ_{ij} is the elastic potential associated with $\mathbf{F}_{ij}$.

The derivatives behave as: $\frac{\partial}{\partial \mathbf{p}_j} = \frac{\tau_i}{mr_0}\frac{\partial}{\partial \mathbf{p}_j^*}, \frac{\partial}{\partial t} = \frac{1}{\tau_i}\frac{\partial}{\partial s}, \frac{\partial}{\partial \mathbf{r}_j} = \frac{1}{r_0}\frac{\partial}{\partial \mathbf{r}_j^*}$.

3.3 The generalized BBGKY hierarchy

A classical system is completely described by a set of initial conditions in phase space and the corresponding Liouville equation. In principle, the solution of the latter gives the temporal behavior of the system. Unfortunately, the extremely large number of internal degrees of freedom present in a grain makes it extremely hard to take into account the evolution of the whole system (internal plus external degrees of freedom).

In the previous section, we obtained a Fokker-Planck equation (3.12) that describes the behavior of the slow external degrees of freedom by means of averaging out the fast behavior of the internal degrees of freedom. That equation is equivalent to a hierarchy of equations, a generalized BBGKY hierarchy, that describe the reduced distributions of degrees of freedom[15, 32].

In order to obtain the generalized BBGKY hierarchy, we need to define the reduced distributions $f^{(n)} \equiv f^{(n)}(X_1, .., X_n, t)$,

$$f^{(n)} = \frac{N!}{(N-n)!}\int dX_{n+1} \cdot dX_N W(X_t, t), \tag{3.13}$$

where $X_i \equiv (\mathbf{r}_i, \mathbf{p}_i)$ and $dX_i \equiv d\mathbf{r}_i d\mathbf{p}_i$.

From the definition of $\mathbf{p}_i^*$, we see that $O(\mathbf{p}_i^*) = 1$. In the strong coupling, short range limit, $O(\phi_{ij}) = mv_g^2$, which implies that $O(\mathbf{F}_{ij}^*) = \frac{r_0}{L}$, where L is the typical deformation of the grain during a collision. In the case of γ_{ij}^*, we have to use the fact that[12]

$$O(\gamma) = \frac{k_B T \tau_v \phi}{L^2},$$

where τ_v is a typical relaxation time for the granular material. We obtain then

$$O(\gamma^*) = T^* \frac{\tau_v \tau_i}{\tau_c^2}.$$

We also have $O(\mathbf{X}_i^*) = 1$. The integrals on X_{n+1} on equation (3.15) are of order nr_0^3.

We can also set the time scale to τ_c, $t = \tau_c s$, in which the interparticle interaction will be of order one.

By integrating equation (3.12), we obtain[16]

$$\begin{aligned}
\frac{\partial}{\partial s} f^{(n)*} = & -\lambda^* \sum_{i=1}^{n} \mathbf{p}_i^* \cdot \frac{\partial}{\partial \mathbf{r}_i^*} f^{(n)*} \\
& - \sum_{i=1}^{n} \sum_{j \neq i}^{n} \bar{\mathbf{F}}_{ij}^* \cdot \frac{\partial}{\partial \mathbf{p}_i^*} f^{(n)*} - g^* \sum_{i=1}^{n} \hat{g} \cdot \frac{\partial}{\partial \mathbf{p}_i^*} f^{(n)*} + \\
& + \frac{\theta}{2} \sum_{j}^{n} \sum_{j \neq k}^{n} \gamma_{jk}^* \hat{\mathbf{r}}_{jk} \hat{\mathbf{r}}_{jk} : \left(\frac{\partial}{\partial \mathbf{p}_j^*} - \frac{\partial}{\partial \mathbf{p}_k^*} \right) \times \\
& \left(T^* \left[\frac{\partial}{\partial \mathbf{p}_j^*} - \frac{\partial}{\partial \mathbf{p}_k^*} \right] + \mathbf{p}_j^* - \mathbf{p}_k^* \right) f^{(n)*} \\
& - n^* \sum_{i=1}^{n} \int dX_{n+1}^* \bar{\mathbf{F}}_{i,n+1}^* \cdot \frac{\partial}{\partial \mathbf{p}_i^*} f^{(n+1)*} + \\
& + \theta n^* \sum_{i=1}^{n} \int dX_{n+1}^* \bar{\gamma}_{i,n+1}^* \hat{\mathbf{r}}_{i,n+1} \hat{\mathbf{r}}_{i,n+1} : \\
& : \frac{\partial}{\partial \mathbf{p}_i^*} \left(T^* \frac{\partial}{\partial \mathbf{p}_i^*} + \mathbf{p}_i^* - \mathbf{p}_{n+1}^* \right) f^{(n+1)*},
\end{aligned} \tag{3.14}$$

where g^* is the normalized value for the gravitational field, $g^* = \frac{gL}{v_g^2}$, $\lambda^* = \frac{\lambda L}{r_0}$, $s = \frac{t}{\tau_c}$ $\theta = \frac{\tau_v}{\tau_c}$ and $n^* = nr_0^3$

3.4 Order of Magnitude of the BBGKY terms

The time-scale for the variation of the distributions $f^{(n)*}$, is set with respect to the time scale τ_c, the duration of a collision. We observe that the most important term for $f^{(n\geq 2)*}$ is the one that corresponds to the direct interaction of the colliding particles, which happens at the time-scale τ_c.

The time-scale λ^* (g^*) corresponds to the time in which density inhomogeneities are smoothed out. The time-scale θ correspond to the time a typical grain needs to interact with another grain in order to lose all its kinetic energy. The time-scale n^* corresponds to the rate of change that synchronizes the multibody distribution to the one body distribution and $n^*\theta$ is the rate of dissipation of kinetic energy.

Reverting to the fully dimensional form for the hierarchy, we define the operators

$$\begin{aligned}
G^n &= \sum_{i=1}^{n} m\mathbf{g}\cdot\frac{\partial}{\partial \mathbf{p}_i}, \\
K^n &= \sum_{i=1}^{n} \frac{\mathbf{p}_i}{m}\cdot\frac{\partial}{\partial \mathbf{r}_i}, \\
I^n &= \sum_{j<i}^{n} \bar{\mathbf{F}}_{ij}\cdot\frac{\partial}{\partial \mathbf{p}_i}, \\
L^n &= \sum_{i=1}^{n} \int dX_{n+1}\bar{\mathbf{F}}_{i,n+1}\cdot\frac{\partial}{\partial \mathbf{p}_i}, \\
M^n &= \frac{1}{2}\sum_{j}^{n}\sum_{j\neq k}^{n} \gamma_{jk}\hat{\mathbf{r}}_{jk}\hat{\mathbf{r}}_{jk} : \left(\frac{\partial}{\partial \mathbf{p}_j} - \frac{\partial}{\partial \mathbf{p}_k}\right) \times \\
&\quad \left(\frac{\partial}{\partial \mathbf{p}_j} - \frac{\partial}{\partial \mathbf{p}_k} + \frac{1}{mk_BT}\left[\mathbf{p}_j - \mathbf{p}_k\right]\right), \\
N^n &= \sum_{i=1}^{n} \int dX_{n+1}\gamma_{i,n+1}\hat{\mathbf{r}}_{i,n+1}\hat{\mathbf{r}}_{i,n+1} : \\
&\quad : \frac{\partial}{\partial \mathbf{p}_i}\left(\frac{\partial}{\partial \mathbf{p}_i} + \frac{1}{mk_BT}\left[\mathbf{p}_i - \mathbf{p}_{n+1}\right]\right),
\end{aligned}$$

where $I^1 = M^1 = 0$. We also define $H^n = K^n + I^n$.

We can now write equation (3.15)

$$\frac{\partial}{\partial s} f^{(n)} = -\lambda^* K^n f^{(n)} - I^n f^{(n)}$$

$$
\begin{aligned}
&-g^* G^n f^{(n)} + \theta M^n f^{(n)} \\
&-n^* L^n f^{(n+1)} + \theta n^* N^n f^{(n+1)},
\end{aligned}
\tag{3.15}
$$

where the different magnitude of each term is made explicit.

3.5 Equations for the one-body and the two-body distribution

As a first step, we rewrite equation (3.15) for f^1 and f^2:

$$
\begin{aligned}
\frac{\partial}{\partial s} f^1 \;=\; & -\lambda^* \frac{\mathbf{p}_1}{m} . \frac{\partial}{\partial \mathbf{r}_1} f^1 - g^* \hat{g} . \frac{\partial}{\partial \mathbf{r}_1} f^1 + \\
& -n^* \int dX_2 \mathbf{F}_{12} . \frac{\partial}{\partial \mathbf{p}_1} f^2 + \\
& +\theta n^* \int dX_2 \gamma_{12} \hat{\mathbf{r}}_{12} \hat{\mathbf{r}}_{12} : \\
& : \frac{\partial}{\partial \mathbf{p}_1} \left(\frac{\partial}{\partial \mathbf{p}_1} + \frac{1}{m k_B T} [\mathbf{p}_1 - \mathbf{p}_2] \right) f,
\end{aligned}
\tag{3.16}
$$

and

$$
\begin{aligned}
\frac{\partial}{\partial s} f^2 \;=\; & -\lambda'^* \left(\frac{\mathbf{p}_1}{m} . \frac{\partial}{\partial \mathbf{r}_1} + \frac{\mathbf{p}_2}{m} . \frac{\partial}{\partial \mathbf{r}_2} \right) f^2 \\
& -\mathbf{F}_{12} . \left(\frac{\partial}{\partial \mathbf{p}_1} - \frac{\partial}{\partial \mathbf{p}_2} \right) f^2 \\
& -g^* m \mathbf{g} . \left(\frac{\partial}{\partial \mathbf{p}_1} + \frac{\partial}{\partial \mathbf{p}_2} \right) f^2 + \\
& +\theta \gamma_{12} \hat{\mathbf{r}}_{12} \hat{\mathbf{r}}_{12} : \left(\frac{\partial}{\partial \mathbf{p}_1} - \frac{\partial}{\partial \mathbf{p}_2} \right) \times \\
& \left(\frac{\partial}{\partial \mathbf{p}_1} - \frac{\partial}{\partial \mathbf{p}_2} + \frac{1}{m k_B T} [\mathbf{p}_1 - \mathbf{p}_2] \right) f^2 - \\
& -n^* \int dX_3 \mathbf{F}_{13} . \frac{\partial}{\partial \mathbf{p}_1} f^3 \\
& -n^* \int dX_3 \mathbf{F}_{23} . \frac{\partial}{\partial \mathbf{p}_2} f^3 + \\
& +\theta n^* \int dX_3 \gamma_{13} \hat{\mathbf{r}}_{13} \hat{\mathbf{r}}_{13} :
\end{aligned}
$$

$$
\begin{aligned}
&: \frac{\partial}{\partial \mathbf{p}_1}\left(\frac{\partial}{\partial \mathbf{p}_1} + \frac{1}{mk_BT}\left[\mathbf{p}_1 - \mathbf{p}_3\right]\right) f^3 + \\
&+\theta n^* \int dX_3 \gamma_{23} \hat{\mathbf{r}}_{23} \hat{\mathbf{r}}_{23} : \\
&: \frac{\partial}{\partial \mathbf{p}_2}\left(\frac{\partial}{\partial \mathbf{p}_2} + \frac{1}{mk_BT}\left[\mathbf{p}_2 - \mathbf{p}_3\right]\right) f^3. \qquad (3.17)
\end{aligned}
$$

The small parameter λ^*, associated with the variations in the density, will be assumed to be very small. Realistically, since $L \approx 10^{-5,-6}$m, $v_g \approx 10^0$m/s and $g \approx 10^1 \text{m}/s^2$, the factor g^*,

$$
g^* = \frac{gL}{v_g^2} \approx 10^{-4,-5}.
$$

We also assume $n^* \approx 10^{-3}$ (for a dilute granular gas) and $\theta \approx 10^{-2}$ (corresponding to a total dissipation of the order of a few percentage points of the total kinetic energy of the grains during a collision). It is natural to assume that $\lambda^* \approx g^* \ll n^* \ll \theta$.

For simplicity, let's assume that $\lambda^* = \alpha g^*$, where $\alpha = O(1)$. We are left with 3 small parameters: λ^* (small gradients), n^* (small density) and θ (small dissipation).

We can now rewrite equations (3.16) and (3.17):

$$
\begin{aligned}
\frac{\partial}{\partial s} f^{1*} &= -\lambda^*(K^1 + G^1) f^{1*} - n^* L^1 f^{2*} + n^* \theta N^1 f^{2*}, \\
\frac{\partial}{\partial s} f^{2*} &= -H^2 f^{2*} - \lambda^* G^2 f^{2*} + \theta M^2 f^{2*} - n^* L^2 f^{3*} \\
&\quad + n^* \theta N^2 f^{3*}.
\end{aligned}
$$

Above, we used the fact that we can assume $\lambda'^* = O(1)$ in this time scale. The evolution of f^{2*} is set by both the interaction (through the operator containing the force) and the kinetics (through the kinetic part of the operator above).

3.6 Extension of the Time Variable

Equation (3.15) cannot be simply solved by a perturbative expansion of the distributions f^n. The reason is that secular terms will appear in the expansion, limiting the validity of the expansions. In order to eliminate these terms, we are going to use the method of extending the time variable s.

We have basically three small expansion parameters: θ (dissipation during a collision); n^*(rate of mixing); λ^*(diffusional). The extension of the time variable is done in the following way $\tau_0 = s$, $\tau_1 = \theta s$, $\tau_2 = n^* s$, $\tau_3 = \lambda^* s$, $\tau_4 = \theta^2 s$, $\tau_5 = n^* \theta s$, etc.

A function $f(s)$ is thus extended into a function of the variables τ_i, $f(s) \equiv f(\tau_0, \tau_1, \tau_2, \tau_3, \tau_4, \tau_5, ...)$. The final dependence in the time variable is obtained, after solving the extended problem, by substituting the τ_i variables by their true dependence on the time variable s. The next step is to do an extension of range of the time variable[33, 16]. The basic idea is to obtain the kinetic behavior of the system (if it exists) and to separate each phenomena according to the time-scale in which they occur[33, 34].

The time derivative becomes

$$\begin{aligned}\frac{\partial}{\partial s} &= \frac{\partial}{\partial \tau_0} + \theta \frac{\partial}{\partial \tau_1} + n^* \frac{\partial}{\partial \tau_2} + \\ & \lambda^* \frac{\partial}{\partial \tau_3} + \theta^2 \frac{\partial}{\partial \tau_4} + n^* \theta \frac{\partial}{\partial \tau_5} + ... \end{aligned} \tag{3.18}$$

Our goal is to decouple the BBGKY system and at the same time avoid secular behavior that limits the validity of our expansions.

By expanding equation (3.15), using the method mentioned above, we obtain for f^{1*}, in the successive orders of magnitude,

$$\frac{\partial}{\partial \tau_0} f_0^1 = 0, \tag{3.19}$$

$$\frac{\partial}{\partial \tau_0} f_1^1 + \frac{\partial}{\partial \tau_1} f_0^1 = 0, \tag{3.20}$$

$$\frac{\partial}{\partial \tau_0} f_2^1 + \frac{\partial}{\partial \tau_2} f_0^1 = -L^1 f_0^2, \tag{3.21}$$

$$\frac{\partial}{\partial \tau_0} f_3^1 + \frac{\partial}{\partial \tau_3} f_0^1 = -(K^1 + G^1) f_0^1, \tag{3.22}$$

$$\frac{\partial}{\partial \tau_0} f_4^1 + \frac{\partial}{\partial \tau_1} f_1^1 + \frac{\partial}{\partial \tau_4} f_0^1 = 0, \tag{3.23}$$

$$\begin{aligned}&\frac{\partial}{\partial \tau_0} f_5^1 + \frac{\partial}{\partial \tau_1} f_2^1 + \\ &+ \frac{\partial}{\partial \tau_2} f_1^1 + \frac{\partial}{\partial \tau_5} f_0^1 = -L^1 f_1^2 + N^1 f_0^2, \end{aligned} \tag{3.24}$$

and for f^{2*}

$$
\begin{aligned}
\frac{\partial}{\partial \tau_0} f_0^2 &= -H^2 f_0^2, && (3.25)\\
\frac{\partial}{\partial \tau_0} f_1^2 + \frac{\partial}{\partial \tau_1} f_0^2 &= -H^2 f_1^2 + M^2 f_0^2, && (3.26)
\end{aligned}
$$

and for f^{3*}

$$
\begin{aligned}
\frac{\partial}{\partial \tau_0} f_3^1 &= -H^3 f_0^3, && (3.27)\\
\frac{\partial}{\partial \tau_0} f_1^3 + \frac{\partial}{\partial \tau_1} f_0^3 &= -H^3 f_1^3 + M^3 f_0^3, && (3.28)
\end{aligned}
$$

A convenient set of initial conditions is given in the next section.

3.7 Initial Conditions

We want to obtain kinetic equations of motion for the distributions f_i^n, in other words,

$$\frac{\partial}{\partial \tau_j} f_0^1 = \phi(f_0^1) + O(\text{higher order}),$$

where $\phi(f_0^1)$ is a function of f_0^1. The multibody distributions, $f_0^{n \geq 2}$ will also be synchronized to f_0^1.

We need, in special, to find the solutions for the equations (3.19-3.28). We assume simple initial conditions, which are not a bad choice, given Grad's theorem [35]. Specifically:

$$
\begin{aligned}
f_0^n(s=0) &= \Pi^n f_0^1,\\
f_0^1(s=0) &= f_0^1,\\
f_i^n(s=0) &= 0 \text{ for } n > 1, i \geq 1,\\
f_i^1(s=0) &= 0 \text{ for } i \geq 1.
\end{aligned}
$$

3.8 Elimination of Secular Terms

In appendix A, we obtain the kinetic equations for the system as consistency conditions by using the method of elimination of secular terms. From equation (3.19) we get that $f_1^1 = 0$ and from equation (3.25), we have

$$f_0^2 = e^{-H^2\tau_0} f_0^2(s=0) = e^{-H^2\tau_0} f_0^1 f_0^1.$$

We also obtain that $f_1^1 = 0$. From equation (3.23) we get that $f_4^1 = 0$ and $f_0^1 \equiv f_0^1(\tau_2, \tau_3, \tau_5)$.

We rewrite equations (A.2), (A.3) and (A.4)

$$\begin{aligned}
\frac{\partial}{\partial \tau_2} f_0^1 &= -L^1 S_{12} f_0^1 f_0^1, \\
\frac{\partial}{\partial \tau_3} f_0^1 &= -(K^1 + G^1) f_0^1, \\
\frac{\partial}{\partial \tau_5} f_0^1 &= +N^1 S_{12} f_0^1 f_0^1.
\end{aligned}$$

Equations (A.2), (A.3) and (A.4) are the kinetic equations for our model of granular systems. We can write them in a more explicit form as

$$\begin{aligned}
\frac{\partial}{\partial \tau_2} f_0^1 &= \int dX_2 \mathbf{F}_{12} \cdot \frac{\partial}{\partial \mathbf{p}_1} S_{12} f_0^1 f_0^1, \\
&= \int d\mathbf{r}_2 d\mathbf{p}_2 (\frac{\mathbf{p}_1 - \mathbf{p}_2)}{m} \cdot \frac{\partial}{\partial \mathbf{r}_{12}} S_{12} f_0^1 f_0^1, \qquad (3.29) \\
\frac{\partial}{\partial \tau_3} f_0^1 &= -\left(\frac{\mathbf{p}_1}{m} \cdot \frac{\partial}{\partial \mathbf{r}_1} + m\mathbf{g} \cdot \frac{\partial}{\partial \mathbf{p}_1} \right) f_0^1, \qquad (3.30) \\
\frac{\partial}{\partial \tau_5} f_0^1 &= \int d\mathbf{r}_2 d\mathbf{p}_2 \gamma_{12} \hat{\mathbf{r}}_{12} \hat{\mathbf{r}}_{12} : \\
&\quad : \frac{\partial}{\partial \mathbf{p}_1} \left(\frac{\partial}{\partial \mathbf{p}_1} + \frac{1}{m k_B T} [\mathbf{p}_1 - \mathbf{p}_2] \right) S_{12} f_0^1 f_0^1, \qquad (3.31)
\end{aligned}$$

where, in equation (3.31), we can use the approximation that

$$S_{12} f_0^1 f_0^1 \approx f_0^1 f_0^1 e^{-\frac{\phi_{12}}{T_g}}.$$

In dimensional form, we finally obtain the kinetic equation

$$\begin{aligned}\frac{\partial}{\partial t} f_0^1 + \left(\frac{\mathbf{p}_1}{m}\cdot\frac{\partial}{\partial \mathbf{r}_1} + m\mathbf{g}\cdot\frac{\partial}{\partial \mathbf{p}_1}\right) f_0^1 &= \\ &= \int dX_2 \mathbf{F}_{12}\cdot\frac{\partial}{\partial \mathbf{p}_1} S_{12} f_0^1 f_0^1 \\ &+ \int d\mathbf{r}_2 d\mathbf{p}_2 \gamma_{12} \hat{\mathbf{r}}_{12}\hat{\mathbf{r}}_{12} : \\ &: \frac{\partial}{\partial \mathbf{p}_1}\left(\frac{\partial}{\partial \mathbf{p}_1} + \frac{1}{mk_BT}\left[\mathbf{p}_1 - \mathbf{p}_2\right]\right) S_{12} f_0^1 f_0^1. \end{aligned} \tag{3.32}$$

The equation above is valid in the limit of small density and small kinetic energy dissipation. Our goal in the next chapter is to derive from it the physical behavior of flowing granular systems.

3.9 The Boltzmann Collisional Term

The collision term is of the same form as the usual elastic Boltzmann collision term. The only difference is the presence of an effective force created by the interaction between internal degrees of freedom. For τ_0 large, we have from equation (A.2)

$$\frac{\partial}{\partial \tau_2} f_0^1 = -L^1 S_{12} f_0^1 f_0^1. \tag{3.33}$$

where $S_{12} = \lim_{\tau_0 \to \infty} e^{-H^2 \tau_0}$. Using the definitions of L^1 and S_{12}, we obtain:

$$\frac{\partial}{\partial \tau_2} f_0^1 = \int d\mathbf{x}_2 d\mathbf{p}_2 \mathbf{F}_{12}\cdot\frac{\partial}{\partial \mathbf{p}_1} S_{12} f_0^1 f_0^1. \tag{3.34}$$

Using the property that as $\tau_0 \to \infty$, $K^2 S_{12} f_0^1 f_0^1 \to I^2 S_{12} f_0^1 f_0^1$ we have:

$$\frac{\partial}{\partial \tau_2} f_0^1 = \int d\mathbf{x}_2 d\mathbf{p}_2 \frac{(\mathbf{p}_1 - \mathbf{p}_2)}{m}\cdot\frac{\partial}{\partial \mathbf{x}_{12}} S_{12} f_0^1 f_0^1.$$

Using Bogoliubov's integration scheme[15, 33, 36]:

$$\frac{\partial}{\partial \tau_2} f_0^1 = \int d\mathbf{p}_2 \frac{\mid \mathbf{p}_1 - \mathbf{p}_2 \mid}{m} \int_0^\infty b db \int_0^{2\pi} d\epsilon \int dx \frac{\partial}{\partial x} S_{12} f_0^1 f_0^1.$$

We finally obtain:

$$\begin{aligned}\frac{\partial}{\partial\tau_2}f_0^1 &= \int d\mathbf{p}_2 d\Omega \frac{\mid \mathbf{p}_1-\mathbf{p}_2 \mid}{m}\sigma(\Omega)\left(f_0^1(\mathbf{p}_1')f_0^1(\mathbf{p}_2')-\right.\\ &\left.-f_0^1(\mathbf{p}_1)f_0^1(\mathbf{p}_2)\right),\end{aligned}\tag{3.35}$$

where the collisional cross-section per solid angle is defined as $\sigma(\Omega)d\Omega = bdbd\epsilon$ (see ref.[36]), and $(\mathbf{p}_1', \mathbf{p}_2')$ are the momenta of the grains before the collision that generate $(\mathbf{p}_1, \mathbf{p}_2)$. The collisional term in equation (3.35) is identical with that for elastic systems[15, 32].

3.10 The Dissipative Contribution

We have then (from Eq.(A.4)):

$$\frac{\partial}{\partial\tau_4}f_0^1 = N^1 S_{12} f_0^1 f_0^1.\tag{3.36}$$

Equation (3.36) then becomes:

$$\begin{aligned}\frac{\partial}{\partial\tau_4}f_0^1 &= \int d\mathbf{x}_2 d\mathbf{p}_2 \gamma_{12}\hat{\mathbf{r}}_{12}\hat{\mathbf{r}}_{12} :\\ &: \frac{\partial}{\partial\mathbf{p}_1}\left(\frac{\partial}{\partial\mathbf{p}_1}+\frac{(\mathbf{p}_1-\mathbf{p}_2)}{mk_BT}\right)S_{12}f_0^1 f_0^1.\end{aligned}\tag{3.37}$$

It can be expressed in a Fokker-Planck form:

$$\begin{aligned}\frac{\partial}{\partial\tau_4}f_0^1 = \frac{\partial}{\partial\mathbf{p}_1}\cdot\int d\mathbf{x}_2 d\mathbf{p}_2 \gamma_{12}\hat{\mathbf{r}}_{12}\frac{\hat{\mathbf{r}}_{12}\cdot(\mathbf{p}_1-\mathbf{p}_2)}{m}S_{12}f_0^1 f_0^1\\ +\frac{\partial}{\partial\mathbf{p}_1}\frac{\partial}{\partial\mathbf{p}_1} : \int d\mathbf{x}_2 d\mathbf{p}_2 \gamma_{12}\hat{\mathbf{r}}_{12}\hat{\mathbf{r}}_{12}S_{12}f_0^1 f_0^1.\end{aligned}\tag{3.38}$$

The first term on the RHS above corresponds to an irreversible transfer of energy into the internal degrees of freedom. The second term corresponds to diffusional energy exchange with the internal modes. When the granular temperature,

$$T_g = \frac{3}{2mk_B} < \mathbf{p}^2 > \approx T,$$

the two terms are of the same order.

As for the expression $S_{12} f_0^1 f_0^1$, we have, in the rarified gas limit, for times larger than $\tau_2 = O(1)$,

$$\begin{aligned} S_{12} f_0^1 f_0^1 &= S_{12} f_0^1(\mathbf{p}_1) f_0^1(\mathbf{p}_2), \\ &\approx f_0^1(\mathbf{p}_1) f_0^1(\mathbf{p}_2) e^{-\frac{\phi_{12}}{k_B T_g(\tau_4)}}, \end{aligned}$$

where ϕ_{12} is the elastic potential energy between the grains.

The approximation above is valid because variations from the main term (zero-th order in Enskog's theory) are small (proportional to the gradients of thermodynamic functions). For the inelastic contribution term, we keep only the leading order term in $f_0^1(2)$, in dimensional form[36]

$$f_0^1(\mathbf{p}) \approx n \left(\frac{1}{2\pi m T_g(\tau_4)} \right)^{\frac{3}{2}} e^{-\frac{\mathbf{p}^2}{2mk_B T_g(\tau_4)}}, \tag{3.39}$$

in the dissipative integral.

Equation(3.38) can be approximated by

$$\begin{aligned} \frac{\partial}{\partial \tau_4} f_0^1 &= \frac{\partial}{\partial \mathbf{p}_1} \cdot \left(f_0^1 \mathbf{p}_1 . \mathbf{A} \right) + \\ &+ \frac{T}{T_g(\tau_4)} \frac{\partial}{\partial \mathbf{p}_1} \frac{\partial}{\partial \mathbf{p}_1} : \left(f_0^1 \mathbf{A} \right), \end{aligned} \tag{3.40}$$

where

$$\mathbf{A} = \int d\hat{\mathbf{r}} \int dr \gamma(r) \hat{\mathbf{r}} \hat{\mathbf{r}} e^{-\frac{\phi(r)}{k_B T_g(\tau_4)}}.$$

Since

$$\int d\hat{\mathbf{r}} \int \hat{\mathbf{r}} \hat{\mathbf{r}} = \frac{4\pi}{3} I,$$

where I is the unitary tensor of second rank, we have

$$\frac{\partial}{\partial \tau_4} f_0^1 = D(T_g) \frac{\partial}{\partial \mathbf{p}_1} \cdot \left[\frac{\partial}{\partial \mathbf{p}_1} + \frac{1}{m k_B T} \mathbf{p}_1 \right] f_0^1, \tag{3.41}$$

where

$$D(T_g) = \int_0^\infty dr \gamma(r) e^{-\frac{\phi(r)}{T_g(\tau_4)}}.$$

3.11 Discussion

Starting from first principles (the Liouville equation and the derived Fokker-Planck equation for the positions and momenta of the granular particles) for a GS, we obtained a generalized BBGKY hierarchy that describe the multi-granular distributions.

Using the small parameters of the theory (small gradients of slow variables, small density and small inelastic dissipation coefficient) we use the methods of perturbation theory and time extension in the several physical time-scales of the problem to open the problem: we obtain the behavior of each term in perturbation theory and eliminate the secular (diverging) terms up to the maximum order possible.

The kinetic equations that describe the time evolution of the one-body distribution are obtained as consistency conditions in the process above described. We recover the standard Boltzmann collisional term and a new collisional term that describes the rate of dissipation of energy.

Chapter 4

The Homogeneous Granular Gas

4.1 Introduction

Recently, granular materials have become the object of much attention[1]: on a practical level, many industrial processes deal with grains or powders (pharmaceutical industries, storage and transport of grains, transport of mineral ore, etc); geophysical phenomena like sand dunes motion, landslides, etc, also correspond to flow of granular particles; on a more abstract level, granular systems are exceptionally rich in terms of the non-equilibrium phenomena they present: kinetic energy dissipation[22]; solid-like to liquid-like transition[37]; dilatancy[38]; arching, and many more[37, 39].

The goal of the present work is to develop kinetic equations for the homogeneous, smooth rarified granular gas based on the kinetic theory methods developed in the previous sections.

We show that these equations obey a generalized H-theorem that works well up to the time-scale that describes the rate of dissipation of kinetic energy.

We will also study the behavior of the granular temperature with respect to time, for the homogeneous solution. The choice of a homogeneous solution is valid as long as we are careful to restrict the system's size so that effects of instability of the homogeneous state will not be important for a small rate of dissipation[40, 41].

4.2 Form For The Potential

The interaction potential corresponds to the elastic (Hertzian) interaction due to the elastic deformation of the grains. We assume that no permanent plastic deformations occur; in other words, the collisions happen slowly compared with the speeds necessary to reach the plastic deformation threshold. For spherical grains, the potential is of the form [28]

$$\phi_{12} = \frac{1}{2} k h^{\frac{5}{2}}, \tag{4.1}$$

where k is an effective elastic constant and $h = 2r_0 - r_{12}$, when $0 < r_{12} < 2r_0$. The restoring force between the grains is then [28]

$$\mathbf{F}_r = \frac{5}{4} k \hat{\mathbf{r}}_{12} h^{\frac{3}{2}}. \tag{4.2}$$

Using a simple classical harmonic crystal approximation, one can obtain the form for the dissipative coefficient $\gamma_{12}(h)$ [12], which can also be obtained by other phenomenological approaches [9, 10]. The radial frictional force between the particles is given by

$$\mathbf{F}_f = \frac{5}{4} k' \hat{\mathbf{r}}_{12} h^{\frac{1}{2}} \dot{h},$$

where k' is a dissipative coefficient. That gives us [12, 10, 9]

$$\frac{\gamma_{12}(h)}{k_B T} = \frac{5}{4} k' h^{\frac{1}{2}}. \tag{4.3}$$

The order of magnitude of $\gamma_{12}(h)$ is[12]

$$\gamma = \frac{k_B T \tau_\nu \phi}{L^2}.$$

4.3 H-Function

If the kinetic energy lost during a collision between two granular particles is a small fraction of the total kinetic energy, then, there should be a function that measures the disorder present in the system. A natural candidate is the generalization of the Boltzmann H-function.

Let's define:

$$H = \int d\mathbf{x}_1 d\mathbf{p}_1 f^1 \log f^1. \tag{4.4}$$

After a few collisional times, $\tau_1 \sim O(1)$, $\frac{\partial}{\partial \tau_0} f_2^1 \approx \frac{\partial}{\partial \tau_0} f_4^1 \approx 0$, and we can write

$$H \approx \int d\mathbf{x}_1 d\mathbf{p}_1 f_0^1 \log f_0^1. \tag{4.5}$$

The time variation of H is given by

$$\frac{\partial}{\partial t} H = n^* \frac{\partial}{\partial \tau_2} H + n^* \theta \frac{\partial}{\partial \tau_4} H. \tag{4.6}$$

The first term will give the usual negative-definite result. For the second term we have:

$$\begin{aligned} \frac{\partial}{\partial \tau_4} H &= \int d\mathbf{x}_1 d\mathbf{p}_1 \frac{\partial}{\partial \tau_4} f_0^1(1)(1 + \log f_0^1(2)); \\ &= \int d\mathbf{x}_1 d\mathbf{p}_1 d\mathbf{r}_{12} d\mathbf{p}_2 (1 + \log f_0^1(2)) \times \\ & \quad \gamma_{12} \hat{\mathbf{r}}_{12} \hat{\mathbf{r}}_{12} : \left(\frac{\partial}{\partial \mathbf{p}_1} - \frac{\partial}{\partial \mathbf{p}_2} \right) \times \\ & \quad \left(\left(\frac{\partial}{\partial \mathbf{p}_1} - \frac{\partial}{\partial \mathbf{p}_2} \right) + \frac{(\mathbf{p}_1 - \mathbf{p}_2)}{m k_B T} \right) S_{12} f_0^1 f_0^1. \end{aligned} \tag{4.7}$$

The equation above can be approximated as before using equation (3.39). Then, we can write:

$$\begin{aligned} \frac{\partial}{\partial \tau_4} H &= \frac{1}{2} \int d\mathbf{x}_1 d\mathbf{p}_1 d\mathbf{x}_2 d\mathbf{p}_2 (2 + \log f_0^1(2) f_0^1(1)) \times \\ & \quad \gamma_{12} \hat{\mathbf{r}}_{12} \hat{\mathbf{r}}_{12} : \left(\frac{\partial}{\partial \mathbf{p}_1} - \frac{\partial}{\partial \mathbf{p}_2} \right) \times \\ & \quad \left(\left(\frac{\partial}{\partial \mathbf{p}_1} - \frac{\partial}{\partial \mathbf{p}_2} \right) + \frac{(\mathbf{p}_1 - \mathbf{p}_2)}{m k_B T} \right) S_{12} f_0^1 f_0^1. \end{aligned} \tag{4.8}$$

Integrating by parts we obtain:

$$\begin{aligned}\frac{\partial}{\partial\tau_4}H \;&\approx\; -\frac{1}{2}\int d\mathbf{x}_1 d\mathbf{p}_1 d\mathbf{x}_2 d\mathbf{p}_2 \frac{\gamma_{12}}{(f_0^1(2)f_0^1(1))}\hat{\mathbf{r}}_{12}\hat{\mathbf{r}}_{12} : \\ &\left(\frac{1}{k_BT}-\frac{1}{k_BT_g(\tau_4)}\right)\frac{(\mathbf{p}_1-\mathbf{p}_2)}{m}(S_{12}f_0^1f_0^1)\times \\ &\left(\frac{\partial}{\partial\mathbf{p}_1}-\frac{\partial}{\partial\mathbf{p}_2}\right)(f_0^1(2)f_0^1(1)),\end{aligned} \tag{4.9}$$

thus giving in fully dimensional form

$$\begin{aligned}\frac{\partial}{\partial\tau_4}H \;&\approx\; -\left(\frac{1}{k_BT}-\frac{1}{k_BT_g(\tau_4)}\right)\frac{1}{k_BT_g(\tau_4)}\times \\ &\int d\mathbf{x}_1 d\mathbf{p}_1 d\mathbf{x}_2 d\mathbf{p}_2\gamma_{12}\left[\hat{\mathbf{r}}_{12}\cdot\frac{(\mathbf{p}_1-\mathbf{p}_2)}{m}\right]^2 S_{12}f_0^1f_0^1\end{aligned} \tag{4.10}$$

We observe that H is a monotonically decreasing function of time, up to the time when $T_g(\tau_4)\sim T$.

4.4 Time Dependence of the Granular Temperature

For the homogeneous system, energy dissipation translates into a decrease of granular temperature. The Boltzmann collision term is conservative so only the friction term will contribute to energy loss. Substituting of equation (3.39) into equation (3.38) yields (in dimensional form, $\gamma_{12}=\frac{5}{4}k'h^{\frac{1}{2}}$)

$$\begin{aligned}\frac{\partial}{\partial\tau_4}f_0^1 \;&\approx\; \int d\mathbf{r}_{12}d\mathbf{p}_2\gamma_{12}\hat{\mathbf{r}}_{12}\hat{\mathbf{r}}_{12} : \\ &:\frac{\partial}{\partial\mathbf{p}_1}\left(\frac{\partial}{\partial\mathbf{p}_1}+\frac{1}{mk_BT}(\mathbf{p}_1-\mathbf{p}_2)\right)S_{12}f_0^1f_0^1, \\ &\approx\; f_0^1\frac{1}{m}\left(\frac{1}{k_BT}-\frac{1}{k_BT_g(\tau_4)}\right)\int d\mathbf{r}_{12}d\mathbf{p}_2\gamma_{12}\times\end{aligned}$$

$$
\begin{aligned}
& \left(1 - \frac{(\mathbf{p}_1.\hat{\mathbf{r}}_{12})^2}{mk_B T_g(\tau_4)}\right) \left(\frac{1}{2\pi m T_g(\tau_4)}\right)^{3/2} \times \\
& e^{-\frac{\mathbf{p}_2^2 + kh^{\frac{5}{2}}}{2} \frac{1}{mk_B T_g(\tau_4)}}, \\
\approx \; & f_0^1 \frac{1}{m} \left(\frac{1}{k_B T} - \frac{1}{k_B T_g(\tau_4)}\right) \times \\
& 4\pi \left(1 - \frac{p_1^2}{3mk_B T_g(\tau_4)}\right) \int_0^{\frac{r_0}{L}} dh \gamma_{12} e^{-\frac{kh^{\frac{5}{2}}}{2k_B T_g(\tau_4)}}.
\end{aligned}
$$

Using the fact that

$$
\frac{\partial}{\partial \tau_4} f_0^1 = -f_0^1 \frac{3}{2T_g(\tau_4)} \left(1 - \frac{p_1^2}{3mk_B T_g(\tau_4)}\right) \frac{\partial}{\partial \tau_4} T_g(\tau_4),
$$

we have:

$$
\begin{aligned}
\frac{\partial}{\partial \tau_4} T_g(\tau_4) = & -\frac{8\pi}{3} \frac{T_g}{m}(\tau_4) \left(\frac{1}{k_B T} - \frac{1}{k_B T_g(\tau_4)}\right) \times \\
& \int_0^\infty dh \frac{5}{4} k' h^{\frac{1}{2}} e^{-\frac{kh^{\frac{5}{2}}}{2k_B T_g(\tau_4)}}. \qquad (4.11)
\end{aligned}
$$

The integral becomes

$$
\int_0^\infty dh \frac{5}{4} k' h^{\frac{1}{2}} e^{-h^{\frac{5}{2}} \frac{1}{2k_B T_g(\tau_4)}} \approx k' \frac{5}{4} \left(\frac{2k_B T_g(\tau_4)}{k}\right)^{\frac{3}{5}} \Gamma(\frac{3}{5}).
$$

We then have

$$
\begin{aligned}
\frac{\partial}{\partial \tau_4} T_g(\tau_4) = & -\frac{10\pi}{3} \left(\frac{2k_B}{k}\right)^{\frac{3}{5}} \Gamma(\frac{3}{5}) \times \\
& \frac{k'}{m} \left(\frac{1}{k_B T} - \frac{1}{k_B T_g(\tau_4)}\right) T_g(\tau_4)^{\frac{8}{5}}, \qquad (4.12)
\end{aligned}
$$

from which we obtain (for $T_g(\tau_4) \gg T$)

$$
T_g(\tau_4) = \frac{T_g(0)}{\left(1 + \frac{10\pi k'}{3mk_B T} \left(\frac{2k_B}{k}\right)^{\frac{3}{5}} \Gamma(\frac{3}{5}) \tau_4\right)^{\frac{5}{3}}}. \qquad (4.13)
$$

We observe that for $T_g(\tau_4) \gg T$, and for long times ($\tau_4 \to \infty$), we have $\dot{T}_g(\tau_4) \propto$

$T_g(\tau_4)^{-\frac{8}{3}}$ and $T_g(\tau_4) \propto \tau_4^{-\frac{5}{3}}$. The exponent $\frac{5}{3}$ compares to the value 2 obtained by assuming a constant phenomenological coefficient of restitution, as we see below.

From a heuristic method in which use of a constant coefficient of restitution is made, one obtains for a one-dimensional granular gas [42]

$$\begin{aligned}\frac{\partial}{\partial t} f^1 &\approx \\ &-\frac{\partial}{\partial p_1} \cdot \left(q f^1(1) \int dp_2 \mid p_1 - p_2 \mid (p_1 - p_2) f^1(2) \right), \qquad (4.14)\end{aligned}$$

with a similar form for three dimensional granular gases.

Using the gaussian approximation for the one-particle distribution functions above, one obtains that the time variation for the granular temperature is given by $\dot{T}_g \propto -T_g^{\frac{3}{2}}$. The solution of which gives $T_g(\tau_4) \propto \tau_4^{-2}$, for large τ_4.

4.5 Discussion

Based on the kinetic equations for the GS derived earlier, we study the behavior of the granular temperature for the case of the homogeneous rarified GG, in the limit of small dissipation.

We derive an appropriate H-theorem for the system and use it to show that the one-body distribution tend to a Maxwellian form on the time scale of the collision rate. Furthermore, it is also shown that the H-theorem is well defined up to the point when the granular temperature becomes comparable with the internal temperature of the grains.

We then obtain the behavior of the granular temperature as a function of time. We compare its assimptotic behavior with that obtained using phenomenological theories that make use of a coefficient of restitution for the granular collision.

Chapter 5

Hydrodynamic Behavior for the Low Density Granular Gas

5.1 Introduction

The goal of this section is to obtain the hydrodynamic behavior of the slow variables (not all conserved) of the GS. We extend the methods of the previous section in order to include the gradients in the system.

Other authors have developed hydrodynamic and kinetic equations for granular flow[2, 42]. They were obtained by assuming an effective interaction between the grains (elastic and frictional forces) [2, 42] that average out the actual stochastic interactions between the grains. The advantage of the present method is that the stochastic interactions due to the existence of the internal degrees of freedom are naturally taken into account from the beginning[13].

5.2 Hydrodynamic Quantities

We can use hydrodynamic methods for the analysis of GS, if we understand its limitations. There are many problems associated with taking the low wave-number limit of the conserved quantities', among them [2]: the length associated with fluctuations of density are comparable with the size of the particles since the particles are large (in some situations, comparable with the container's length, as in large grains flowing through a pipe); kinetic energy is irreversibly dissipated during a collision; With that in mind, we are going to propose a model that tries to fit the behavior of a rarified granular gas.

Using the solutions of the kinetic equations obtained earlier, we define:

$$\begin{aligned} n(\mathbf{r}_1,s) &= \int d\mathbf{p}_1 f_0^1(\mathbf{r}_1,\mathbf{p}_1,s), && (5.1)\\ \mathbf{u}(\mathbf{r}_1,s) &= \frac{1}{mn}\int d\mathbf{p}_1\mathbf{p}_1 f_0^1(\mathbf{r}_1,\mathbf{p}_1,s), && (5.2)\\ T_g(\mathbf{r}_1,s) &= \frac{1}{3nm}\int d\mathbf{p}_1(\mathbf{p}_1-m\mathbf{u})^2 f_0^1(\mathbf{r}_1,\mathbf{p}_1,s), && (5.3)\end{aligned}$$

where $\mathbf{u}(\mathbf{r}_1,s)$ is the flow vector field, $n(\mathbf{r}_1,s)$ is the density and $T_g(\mathbf{r}_1,s)$ is the granular temperature.

5.2.1 Variation of Density

We have

$$\frac{\partial n}{\partial s} = \int d\mathbf{p}_1\frac{\partial}{\partial s}f_0^1.$$

Using the extension for the time derivative, we obtain

$$\begin{aligned} &\left(\frac{\partial}{\partial\tau_0}+\theta\frac{\partial}{\partial\tau_1}+n^*\frac{\partial}{\partial\tau_2}+\right.\\ &\left.+\lambda^*\frac{\partial}{\partial\tau_3}+\theta^2\frac{\partial}{\partial\tau_4}+n^*\theta\frac{\partial}{\partial\tau_5}\right)n = \\ &= \int d\mathbf{p}_1^*\left(\frac{\partial}{\partial\tau_0}+\ldots+n^*\theta\frac{\partial}{\partial\tau_5}\right)f_0^1. \qquad (5.4)\end{aligned}$$

From above we obtain

$$\begin{aligned} 0=\frac{\partial n}{\partial\tau_0}=\frac{\partial n}{\partial\tau_1} &= \frac{\partial n}{\partial\tau_2}, && (5.5)\\ \frac{\partial n}{\partial\tau_3} &= \int d\mathbf{p}_1\frac{\partial}{\partial\tau_3}f_0^1, && (5.6)\\ 0=\frac{\partial n}{\partial\tau_4} &= \frac{\partial n}{\partial\tau_5}. && (5.7)\end{aligned}$$

We can deduce from above that $n \equiv n(\tau_3)$.

From (5.6) we obtain

$$\begin{aligned}
\frac{\partial n}{\partial \tau_3} &= \int d\mathbf{p}_1 \frac{\partial}{\partial \tau_3} f_0^1, \\
&= -\int d\mathbf{p}_1 \left(\frac{\mathbf{p}_1}{m} \cdot \frac{\partial}{\partial \mathbf{r}_1} + m\mathbf{g} \cdot \frac{\partial}{\partial \mathbf{p}_1} \right) f_0^1, \\
&= -\frac{\partial}{\partial \mathbf{r}_1} \cdot \int d\mathbf{p}_1 \frac{\mathbf{p}_1}{m} f_0^1,
\end{aligned}$$

from which we get

$$\frac{\partial n}{\partial \tau_3} = -\frac{\partial}{\partial \mathbf{r}_1} \cdot (n\mathbf{u}). \tag{5.8}$$

5.2.2 Particle Flow

For a granular system, momentum is a conserved quantity, which is not true for the granular temperature (translational kinetic energy). By taking the time derivative (with respect to s) of equation(5.2), we obtain the variations of $\mathbf{u}$ at all orders of magnitude:

$$\frac{\partial}{\partial \tau_0}(n\mathbf{u}) = 0, \tag{5.9}$$

$$\frac{\partial}{\partial \tau_1}(n\mathbf{u}) = 0, \tag{5.10}$$

$$\frac{\partial}{\partial \tau_2}(n\mathbf{u}) = \frac{1}{m} \int d\mathbf{p}_1 \mathbf{p}_1 \frac{\partial}{\partial \tau_2} f_0^1, \tag{5.11}$$

$$\frac{\partial}{\partial \tau_3}(n\mathbf{u}) = \frac{1}{m} \int d\mathbf{p}_1 \mathbf{p}_1 \frac{\partial}{\partial \tau_3} f_0^1, \tag{5.12}$$

$$\frac{\partial}{\partial \tau_4}(n\mathbf{u}) = 0, \tag{5.13}$$

$$\frac{\partial}{\partial \tau_5}(n\mathbf{u}) = \frac{1}{m} \int d\mathbf{p}_1 \mathbf{p}_1 \frac{\partial}{\partial \tau_5} f_0^1. \tag{5.14}$$

From equations (5.9,5.10,5.13), we obtain that $\mathbf{u} \equiv \mathbf{u}(\tau_2, \tau_3, \tau_5)$. From equation (5.11) and the fact that gradients of the density are of order λ^*, we obtain that $\mathbf{u} \equiv \mathbf{u}(\tau_3, \tau_5)$.

Our next step is to analyze the final term

$$\begin{aligned}
\frac{\partial}{\partial \tau_5}\mathbf{u}_0 &= \int d\mathbf{p}_1\mathbf{p}_1\frac{\partial}{\partial \tau_5}f_0^1, \\
&= \int d\mathbf{p}_1\mathbf{p}_1 \int d\mathbf{p}_2 d\mathbf{r}_2\gamma_{12}\hat{\mathbf{r}}_{12}\hat{\mathbf{r}}_{12} : \\
&: \frac{\partial}{\partial \mathbf{p}_1}\left(\frac{\partial}{\partial \mathbf{p}_1} + \frac{1}{mk_BT}\left[\mathbf{p}_1 - \mathbf{p}_2\right]\right) f_0^2
\end{aligned}$$

The integral above is zero due to the symmetries of f_0^2. From that we obtain $\mathbf{u} \equiv \mathbf{u}(\tau_3)$.

Let's define the pressure tensor:

$$\begin{aligned}
\mathbf{P} &= \frac{1}{m}\int d\mathbf{p}_1\left(\mathbf{p}_1 - m\mathbf{u}\right)\left(\mathbf{p}_1 - m\mathbf{u}\right) f_0^1, \\
&= \frac{1}{m}\int d\mathbf{p}_1\mathbf{p}_1\mathbf{p}_1 f_0^1 - nm\mathbf{u}\mathbf{u}. \qquad (5.15)
\end{aligned}$$

We can write equation (5.12) on the detailed form

$$\frac{\partial}{\partial \tau_3}(nm\mathbf{u}) = -\int d\mathbf{p}_1\mathbf{p}_1\left(\frac{\mathbf{p}_1}{m}.\frac{\partial}{\partial \mathbf{r}_1} + m\mathbf{g}.\frac{\partial}{\partial \mathbf{p}_1}\right) f_0^1.$$

The external force integral above gives the value

$$-m\int d\mathbf{p}_1\mathbf{p}_1\mathbf{g}.\frac{\partial}{\partial \mathbf{p}_1}f_0^1 = nm\mathbf{g}.$$

The kinetic part above can be written in the form

$$-\frac{1}{m}\frac{\partial}{\partial \mathbf{r}_1}.\int d\mathbf{p}_1\mathbf{p}_1\mathbf{p}_1 f_0^1 = -\frac{\partial}{\partial \mathbf{r}_1}.\left(\mathbf{P} + nm\mathbf{u}\mathbf{u}\right).$$

We then write

$$\frac{\partial}{\partial \tau_3}\mathbf{u} = -\frac{1}{nm}\frac{\partial}{\partial \mathbf{r}_1}.\mathbf{P} - \mathbf{u}.\frac{\partial}{\partial \mathbf{r}_1}\mathbf{u} + \mathbf{g}\,\cdot \qquad (5.16)$$

5.2.3 Granular Temperature

We define the energy flow vector

$$= \frac{1}{2m^2}\int d\mathbf{p}_1(\mathbf{p}_1 - m\mathbf{u})^2(\mathbf{p}_1 - m\mathbf{u})f_0^1. \qquad (5.17)$$

from which we obtain

$$\begin{aligned}\mathbf{q} &= \frac{1}{2m^2}\int d\mathbf{p}_1 p_1^2\mathbf{p}_1 f_0^1 - \mathbf{u}\cdot\mathbf{P} - \frac{3}{2}n\mathbf{u}T_g \\ &\quad -\frac{1}{2}n\mathbf{u}\mathbf{u}^2,\end{aligned}$$

since from equation (5.3)

$$T_g = \frac{1}{3nm}\int d\mathbf{p}_1 f_0^1 p_1^2 - \frac{m\mathbf{u}^2}{3}.$$

We proceed to investigate the temporal behavior of T_g. We can show that T_g does not depend on τ_0, τ_1, τ_2 or τ_4. The latter happens because the integral

$$\int d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{r}_2\mathbf{p}_1\mathbf{F}_{12}\cdot\frac{\partial}{\partial\mathbf{p}_1}S_{12}f_0^1 f_0^1$$

is of higher order.

We have to calculate the time dependence of T_g on τ_3.

$$\begin{aligned}\frac{\partial}{\partial\tau_3}(nT_g) &= \frac{1}{3}\int d\mathbf{p}_1 p_1^2\frac{\partial}{\partial\tau_3}f_0^1 - \frac{\partial}{\partial\tau_3}\left(\frac{nm\mathbf{u}^2}{3}\right), \\ &= -\frac{1}{3m^2}\frac{\partial}{\partial\mathbf{r}_1}\cdot\int d\mathbf{p}_1 p_1^2\mathbf{p}_1 f_0^1 + \frac{2}{3}nm\mathbf{g}.\mathbf{u} \\ &\quad -\frac{\partial}{\partial\tau_3}\left(\frac{nmu^2}{3}\right).\end{aligned}$$

We obtain from above:

$$\frac{\partial}{\partial\tau_3}(nT_g) = n\frac{\partial}{\partial\tau_3}T_g - T_g\frac{\partial}{\partial\mathbf{r}_1}(n\mathbf{u}),$$

$$\begin{aligned} &= -\frac{1}{3m^2}\frac{\partial}{\partial \mathbf{r}_1}\cdot\int d\mathbf{p}_1 p_1^2 \mathbf{p}_1 f_0^1 + \frac{2}{3}nm\mathbf{g}.\mathbf{u} \\ &\quad -\frac{\partial}{\partial\tau_3}\left(\frac{nu^2}{3}\right). \end{aligned}$$

After substitution and a little algebra, we obtain:

$$\begin{aligned} n_0\frac{\partial}{\partial\tau_3}T_g + n\mathbf{u}.\frac{\partial}{\partial \mathbf{r}_1}T_g &= -\frac{2}{3}\frac{\partial}{\partial \mathbf{r}_1}.\mathbf{q} \\ &\quad -\frac{2}{3}\mathbf{P} : \frac{\partial}{\partial \mathbf{r}_1}\mathbf{u}. \end{aligned} \tag{5.18}$$

The dependence of T_g on τ_5 is given by

$$\begin{aligned} \frac{\partial}{\partial\tau_5}(nT_g) &= \frac{1}{3}\int d\mathbf{p}_1 p_1^2 \frac{\partial}{\partial\tau_5} f_0^1 - \frac{\partial}{\partial\tau_5}\left(\frac{nm\mathbf{u}^2}{3}\right), \\ &= \frac{1}{3}\int d\mathbf{p}_1 p_1^2 \int d\mathbf{p}_2 d\mathbf{r}_2 \gamma_{12}\hat{\mathbf{r}}_{12}\hat{\mathbf{r}}_{12} : \\ &: \frac{\partial}{\partial \mathbf{p}_1}\left(\frac{\partial}{\partial \mathbf{p}_1} + \frac{1}{mk_BT}\left[\mathbf{p}_1 - \mathbf{p}_2\right]\right) S_{12} f_0^1 f_0^1, \end{aligned}$$

where we can use once more that

$$S_{12} f_0^1 f_0^1 \approx f_0^1 f_0^1 e^{-\frac{\phi_{12}}{T_g}},$$

finally obtaining

$$\begin{aligned} \frac{\partial}{\partial\tau_5}(nT_g) &= \frac{1}{3}\int d\mathbf{p}_1 p_1^2 \int d\mathbf{p}_2 d\mathbf{r}_2 \gamma_{12}\hat{\mathbf{r}}_{12}\hat{\mathbf{r}}_{12} : \\ &: \frac{\partial}{\partial \mathbf{p}_1}\left(\frac{\partial}{\partial \mathbf{p}_1} + \frac{1}{mk_BT}\left[\mathbf{p}_1 - \mathbf{p}_2\right]\right) f_0^1 f_0^1 e^{-\frac{\phi_{12}}{T_g}}, \end{aligned}$$

and[16]

$$\begin{aligned} \frac{\partial}{\partial\tau_5}(nT_g(t)) &= -\frac{8\pi n^2\sigma^2}{3}\frac{T_g(t)}{m}\left(\frac{1}{T} - \frac{1}{T_g(t)}\right) \times \\ &\quad \int_0^\infty dh T\gamma(h) e^{-\frac{\phi_{12}(h)}{2T_g(t)}}, \end{aligned} \tag{5.19}$$

where $h = \sigma - r_{12}$ and $\phi_{12}(h)$ is the Hertzian potential between two grains.

Equations (5.8),(5.16),(5.18) and (5.19) define the hydrodynamic behavior of the rarified, quasi-uniform granular gas.

5.3 Solution of the Kinetic Equations

In our search for the behavior of the quasi-homogeneous, rarified granular gas, we have assumed in the previous sections that the gradients of the thermodynamical variables were small compared to the density parameters, $\lambda \ll n^*$. We will expand the solution for equation (3.32) around the zeroth order Enskog solution for the Boltzmann equation (obtained from the above mentioned equations by making $\gamma_{12} \rightarrow 0$)[36].

We write

$$f_0^1 = \varphi_0 + \varphi_0 \varphi_1, \tag{5.20}$$

where φ_0 corresponds to the zeroth order Enskog solution[36].

The order of magnitude of φ_1 is given by

$$O(\varphi_1) = \frac{l_{MF}}{l_G} \approx \frac{r_0}{n^* l_G} \ll 1,$$

showing that the expansion will be valid for small gradients only. It is also important to compare the order above with the magnitude of the rate of dissipation, $n^*\theta$. The solution above will be meaningful in the case when $1 \gg O(\varphi_1) \gg n^*\theta \gg n^{*2}$. We need

$$\frac{1}{n^*}\frac{1}{n^*\theta} \gg \frac{l_G}{r_0} \gg \frac{1}{n^*}.$$

From above, we see that for $\frac{1}{n^*}\frac{1}{n^*\theta} \ll \frac{l_G}{r_0}$, the system may be treated as homogeneous.

We write equation (3.32)

$$\frac{\partial}{\partial t} f_0^1 + K f_0^1 = J(f_0^1 f_0^1) + \Gamma(f_0^1 f_0^1), \tag{5.21}$$

where

$$K f_0^1 = \left(\frac{\mathbf{p}_1}{m} . \frac{\partial}{\partial \mathbf{r}_1} + m\mathbf{g} . \frac{\partial}{\partial \mathbf{p}_1} \right) f_0^1,$$

and

$$J(f_0^1 f_0^1) = \int dX_2 \mathbf{F}_{12} . \frac{\partial}{\partial \mathbf{p}_1} S_{12} f_0^1 f_0^1,$$

and

$$\Gamma(f_0^1 f_0^1) = \int d\mathbf{r}_2 d\mathbf{p}_2 \gamma_{12} \hat{\mathbf{r}}_{12} \hat{\mathbf{r}}_{12} :$$
$$: \frac{\partial}{\partial \mathbf{p}_1} \left(\frac{\partial}{\partial \mathbf{p}_1} + \frac{1}{m k_B T} [\mathbf{p}_1 - \mathbf{p}_2] \right) S_{12} f_0^1 f_0^1 .$$

The function φ_0 is of the order of the density of the system and $O(\varphi_1) \gg \lambda$. In consequence, we assume that φ_1 corresponds to the first order Enskog approximation.

We write then

$$\varphi_0 = \frac{n}{(2\pi m T_g)^{\frac{3}{2}}} \exp\left(-\frac{p_1^2}{2 m T_g} \right), \tag{5.22}$$

and (see appendix B)

$$\varphi_1 = -\frac{1}{n} \left(\frac{2\pi T_g}{m} \right)^{\frac{1}{2}} \mathbf{A} \cdot \frac{\partial}{\partial \mathbf{r}_1} \ln T_g - \frac{2}{n} \mathbf{B} : \frac{\partial}{\partial \mathbf{r}_1} \mathbf{u}, \tag{5.23}$$

where $(O(\mathbf{A}, \mathbf{B}) = \frac{1}{v_g r_0^2})$.

The expressions for the pressure tensor $\mathbf{P}$ and the heat flux vector $\mathbf{q}$ are given by

$$\mathbf{P} = n T_g \mathbf{U} - \eta \left(\frac{\partial}{\partial \mathbf{r}_1} \mathbf{u} + \left[\frac{\partial}{\partial \mathbf{r}_1} \mathbf{u} \right]^{\dagger} - \frac{2}{3} \mathbf{U} \frac{\partial}{\partial \mathbf{r}_1} \cdot \mathbf{u} \right)$$

and

$$\mathbf{q} = -\lambda_T \frac{\partial}{\partial \mathbf{r}_1} T_g,$$

where η is the viscosity coefficient, λ_T is the thermal conductivity coefficient (see appendix B) and $[\mathbf{A}]^{\dagger}$ is the transpose of $\mathbf{A}$

We observe that the only difference, from the usual hydrodynamical equations that we obtain, for the rarified, quasi-homogeneous granular gas, corresponds to the result obtained by Schoffield and Oppenheim in the limit of small gradients[13].

5.4 Linearized granular hydrodynamics

The analysis of stability was done for granular systems has been done by several authors for different models of granular systems[40]. In what follows we use the notation

$$\nabla \equiv \frac{\partial}{\partial \mathbf{r}_1}.$$

5.4.1 Modified Navier-Stokes equations

We will study the effect of dissipation on the long-time behavior of the solution (5.20). In order to do so, let's rewrite the hydrodynamic equations obtained for the rarified, quasi-homogeneous, quasi-elastic granular gas:

$$\begin{aligned}
\frac{\partial n}{\partial t} &= -\nabla.(n\mathbf{u}). && (5.24)\\
\frac{\partial}{\partial t}\mathbf{u} &= -\frac{1}{mn}\nabla(nT_g) \\
&\quad +\nabla\cdot\left(\frac{\eta}{nm}\left(\nabla\mathbf{u}+[\nabla\mathbf{u}]^{\dagger}-\frac{2}{3}\nabla\cdot\mathbf{u}\right)\right) \\
&\quad -\mathbf{u}\cdot\nabla\mathbf{u}+\mathbf{g}, && (5.25)\\
n\frac{\partial}{\partial t}T_g &= -n\mathbf{u}\cdot\nabla T_g+\frac{2}{3}\nabla\cdot(\lambda_T\nabla T_g)-\frac{2}{3}nT_g\nabla\cdot\mathbf{u} \\
&\quad -\eta\left(\nabla\mathbf{u}+[\nabla\mathbf{u}]^{\dagger}\right):\nabla\mathbf{u}-\frac{2\eta}{3}(\nabla\cdot\mathbf{u})^2 \\
&\quad -D(T_g)(1-\frac{k_BT}{T_g}), && (5.26)
\end{aligned}$$

where $\eta \equiv$ shear viscosity, $\lambda_T \equiv$ thermal conductivity,

$$D(T_g) = -\frac{8\pi n^2\sigma^2 T_g}{3m}\int_0^\infty dh\gamma(h)e^{-\frac{\phi_{12}(h)}{2T_g(t)}},$$

and $T_g \gg k_BT$.

Using the forms[12]

$$\gamma(h) = \frac{5}{4}k'h^{\frac{1}{2}},$$

and

$$\phi_{12}(h) = \frac{1}{2}kh^{\frac{3}{2}},$$

we obtain approximatively[16]

$$\begin{aligned} D(T_g) &= -\frac{10\pi n\sigma^2}{3}\left(\frac{2}{k}\right)^{\frac{3}{5}}\Gamma(0.6)\frac{k'}{m}T_g(t)^{\frac{8}{5}} \\ &= -Dk'nT_g(t)^{\frac{8}{5}}. \end{aligned}$$

The results obtained in equations (5.24),(5.25) and (5.26) correspond to those obtained in reference [40] with the absence of the term that in [40] corresponds to higher order, namely $-\nabla n$, which is of order $n^*\theta\lambda$ in the present theory.

For the same reason as above, several terms obtained in reference [13] are ignored for being of higher order.

5.4.2 Linearized Hydrodynamics

We expand the generalized Navier-Stokes equations around the small values defined by

$$\begin{aligned} n &= n_0 + \delta n, \\ \mathbf{u} &= \delta\mathbf{u}, \\ T_g &= T_0 + \delta T, \end{aligned}$$

where the delta variables are the small deviations from the uniform state.

We obtain

$$\begin{aligned} \frac{\partial}{\partial t}\delta n &= -n_0\nabla.(\delta\mathbf{u}). && (5.27) \\ mn_0\frac{\partial}{\partial t}\delta\mathbf{u} &= -n_0\nabla(\delta T) - T_0\nabla(\delta n) \\ &\quad +\eta_0\left(\nabla^2\delta\mathbf{u} - \frac{1}{3}\nabla\nabla\cdot\delta\mathbf{u}\right) + \mathbf{g}, && (5.28) \\ n_0\frac{\partial}{\partial t}\delta T &= +\frac{2\lambda_{T0}}{3}\nabla^2\delta T - \frac{2}{3}n_0T_0\nabla\cdot\delta\mathbf{u} \end{aligned}$$

$$\begin{aligned} & -Dk'T_0(t)^{\frac{8}{5}}\delta n - \frac{8}{5}Dk'n_0T_0(t)^{\frac{3}{5}}\delta T, \\ n_0\frac{\partial}{\partial t}T_0 &= -Dk'n_0T_0^{\frac{8}{5}}. \end{aligned} \tag{5.29}$$

The next step will be to analyze the behavior of the hydrodynamic modes of the system.

5.5 Discussion

In this section, we obtain a set of generalized Navier-Stokes equations for the granular gas. An unusual term, proportional to a power of the granular temperature. is obtained, that reflect the inelastic dissipative behavior of the grains during a collision.

Using a method similar to the one invented by Chapman and Enskog, we solve the kinetic equations obtained earlier and obtain the generalized Navier-Stokes equation for the low density, non-homogeneous GG.

We then study the effect of the inelasticity on the stability of a class of solutions for the behavior of the hydrodynamic (the slow ones: the same as the ones for usual molecular gases) variables of the system.

Chapter 6

Conclusions

In summary, in this Thesis, we study the flow and collisional aspects of granular systems (GS).

We first obtain the coefficient of instantaneous energy dissipation for collisions between two grains by an appropriate separation of the potential energy into internal, granular and coupling parts and with the help of a first principles theory for granular distribution functions.

The form for the dissipative coefficient $\gamma(r)$ that we obtain is identical to the ones obtained elsewhere[9, 10] assuming phenomenological viscoelastic dissipative coefficients. The agreement suggests that the phenomenological model is a plausible one to describe the interaction between GPs that do not involve plastic deformation of the grains.

We then proceed to study the flow aspect of GS. Starting from first principles (the Liouville equation and the derived Fokker-Planck equation for the positions and momenta of the granular particles) for a GS, we obtained a generalized BBGKY hierarchy that describes the multi-granular distributions.

Using the small parameters of the theory (small gradients of slow variables, small density and small inelastic dissipation coefficient) we take advantage of perturbation theory and time extension in the several physical time-scales of the problem to make it tractable: we obtain the behavior of each term in perturbation theory and eliminate the secular (diverging) terms up to the maximum order possible.

The kinetic equations that describe the time evolution of the one-body distribution are obtained as consistency conditions in the process above described. We recover the standard Boltzmann collisional term and a new collisional term that describes the rate of dissipation of energy.

Based on the kinetic equations for the GG derived earlier, we study the behavior of the granular temperature for the case of the homogeneous rarified GG, in the limit of small dissipation.

We derive an appropriate H-theorem for the system and use it to show that the one-body distribution tends to a Maxwellian form on the time scale of the collision rate. Furthermore, it is also shown that the H-theorem is well defined up to the point when the granular temperature becomes comparable with the internal temperature of the grains.

We then obtain the behavior of the granular temperature as a function of time. We compare its asymptotic behavior with that obtained using phenomenological theories that make use of a coefficient of restitution for the granular collision.

In the last section,we obtain a set of generalized Navier-Stokes equations for the granular gas. An unusual term, proportional to a power of the granular temperature, is obtained that reflects the inelastic dissipative behavior of the grains during a collision.

We then use a method similar to the one invented by Chapman and Enskog, in order to solve the kinetic equations obtained earlier and obtain the generalized Navier-Stokes equation for the low density, non-homogeneous GG.

We then study the effect of the inelasticity on the stability of a class of solutions for the behavior of the hydrodynamic (the slow ones: the same as the ones for usual molecular gases) variables of the system.

Appendix A

Elimination of secular behavior from expansions

From equation (3.19), we obtain that $f_0^1 \equiv f_0^1(\tau_1, \tau_2, \tau_3, \tau_4, \tau_5)$. Integrating equation (3.20) with respect to τ_0, we have

$$\begin{aligned} f_1^1(\tau_0) &= f_1^1(\tau_0 = 0) + \tau_0 \frac{\partial f_0^1}{\partial \tau_1}, \\ &= \tau_0 \frac{\partial f_0^1}{\partial \tau_1}. \end{aligned}$$

The behavior of f_1^1 becomes secular when $\tau_0 \to \infty$. Since we can rearrange the terms inside the perturbative expansion of the distributions, we choose f_0^1 such that

$$\frac{\partial f_0^1}{\partial \tau_1} = 0.$$

That implies that $f_1^1 = 0$ and $f_0^1 \equiv f_0^1(\tau_2, \tau_3, \tau_4, \tau_5)$.

We proceed in the same way up to the precision order we want to attain. From equation (3.25), we obtain:

$$\begin{aligned} f_0^2(\tau_0) &= e^{-H_2 \tau_0} f_0^2(0), \\ &= e^{-H_2 \tau_0} f_0^1 f_0^1, \end{aligned} \tag{A.1}$$

and the integration of equation (3.20) with respect to τ_0 gives us

$$\begin{aligned} f_2^1(\tau_0) &= f_2^1(0) - \tau_0 \frac{\partial f_0^1}{\partial \tau_2} - L^1 \int_0^{\tau_0} d\lambda e^{-H_2\lambda} f_0^1 f_0^1 \\ &= -\tau_0 \frac{\partial f_0^1}{\partial \tau_2} - L^1 \int_0^{\tau_0} d\lambda e^{-H_2\lambda} f_0^1 f_0^1 \end{aligned}$$

From equation (3.26), we obtain (after replacing f_0^2 by $e^{-H_2\tau_0} f_0^1 f_0^1$

$$f_1^2 = \int_0^{\tau_0} d\lambda e^{-H^2(\tau_0-\lambda)} M^2 e^{-H^2\lambda} f_0^1 f_0^1.$$

The expression $L^1 \int_0^{\tau_0} d\lambda e^{-H_2\lambda} f_0^1 f_0^1$ diverges when $\tau_0 \to \infty$ because

$$\lim_{\tau_0 \to \infty} e^{-H_2\tau_0} f_0^1 f_0^1 = C_0 \approx e^{-\beta\phi_{12}} f_0^1 f_0^1,$$

where C_0 does not depend on τ_0. In order to remove the secular term above, we write

$$\begin{aligned} L^1 \int_0^{\tau_0} d\lambda e^{-H_2\lambda} f_0^1 f_0^1 &= L^1 \int_0^{\tau_0} d\lambda \left(e^{-H_2\lambda} - S_{12} \right) f_0^1 f_0^1 \\ &\quad + \tau_0 L^1 S_{12} f_0^1 f_0^1, \end{aligned}$$

where $S_{12} = \lim_{\tau_0 \to \infty} e^{-H_2\tau_0}$, and the first term above converges. We then eliminate the secular term on $f_2^1(\tau_0)$ and obtain the consistency equation

$$\frac{\partial f_0^1}{\partial \tau_2} = -L^1 S_{12} f_0^1 f_0^1, \qquad \text{(A.2)}$$

which is equivalent to the Boltzmann collisional term for molecular theories.

From equation (3.22), we obtain

$$f_3^1(\tau_0) = -\tau_0 \left(\frac{\partial f_0^1}{\partial \tau_1} + (K^1 + G^1) f_0^1 \right).$$

The secular term above is eliminated by choosing

$$\frac{\partial f_0^1}{\partial \tau_1} = -(K^1 + G^1) f_0^1. \qquad \text{(A.3)}$$

From (3.23), we obtain $f_4^1 = 0$ and

$$\frac{\partial f_0^1}{\partial \tau_4} = 0.$$

From (3.24), using that

$$\frac{\partial f_2^1}{\partial \tau_1} = 0,$$

we finally obtain, in the limit when $\tau_0 \to \infty$,

$$\begin{aligned} \frac{\partial}{\partial \tau_5} f_0^1 &= \lim_{\tau_0 \to \infty} \left(-L^1 f_1^2 + N^1 f_0^2 \right) \\ &= +N^1 S_{12} f_0^1 f_0^1. \end{aligned} \tag{A.4}$$

Appendix B

Chapman-Enskog results

We rewrite some of the results that can be found in reference [36] for the approximation of f_0^1 in section 10.

The vector **A** is a solution of

$$\begin{aligned} \frac{1}{n}\int d\hat{\mathbf{e}}d\mathbf{c}\alpha_{12}\frac{\mid \mathbf{p}_1 - \mathbf{p}_2 \mid}{m} f_1 f(\mathbf{A'}_1 + \mathbf{A'} - \mathbf{A}_1 - \mathbf{A}) &= \\ &= f\left(\mathcal{C}\cdot\mathcal{C} - \frac{5}{2}\right)\mathcal{C}, \end{aligned} \tag{B.1}$$

where α_{12} is the collisional cross-section, and the normalized peculiar velocity $\mathcal{C}$, is defined by

$$\mathcal{C} = \left(\frac{m}{2T_g}\right)^{\frac{1}{2}}\left(\frac{\mathbf{p}}{\mathbf{m}} - \mathbf{u}\right). \tag{B.2}$$

The vector **A** has the form

$$\mathbf{A} = A(\mid \mathcal{C} \mid)\mathcal{C},$$

where $A(\mid \mathcal{C} \mid)$ is a function of $\mid \mathcal{C} \mid$, n and T_g.

The tensor **B** is a solution of

$$\begin{aligned} \frac{1}{n}\int d\hat{\mathbf{e}}d\mathbf{c}\alpha_{12}\frac{\mid \mathbf{p}_1 - \mathbf{p}_2 \mid}{m} f_1 f(\mathbf{B'}_1 + \mathbf{B'} - \mathbf{B}_1 - \mathbf{B}) &= \\ &= f\left(\mathcal{C}\mathcal{C} - \frac{1}{3}\mathrm{U}\mathcal{C}\cdot\mathcal{C}\right). \end{aligned} \tag{B.3}$$

The tensor **B** has the form

$$\mathbf{B} = B(|\, \mathcal{C} \,|) \left(\mathcal{C}\mathcal{C} - \frac{1}{3}\mathcal{C} \cdot \mathcal{C} \right),$$

where $B(|\, \mathcal{C} \,|)$ is also a function of $|\, \mathcal{C} \,|$, n and T_g.

The results for λ_T and μ_v are

$$\lambda_T = \frac{75}{8} \frac{T_g}{m} \frac{1}{a_{11}}, \tag{B.4}$$

$$\mu_v = \frac{5}{2} T_g \frac{1}{b_{11}}, \tag{B.5}$$

where a_{11} and b_{11} are constants that depend on the system[36].

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