Chapter 2

Kinetic Theory of Granular Gases

2.1 Introduction

The systematic framework for extracting macroscopic information about a gas from microscopic collision dynamics is the kinetic theory of gases (KTG) [1]. The goal of kinetic theory is to set up Boltzmann-Enskog (BE) type equations for a particular model of interaction. The solution of these equations should give either the equilibrium state solution of the system, or it should describe the approach of the distribution function to the asymptotic state [2, 3].

The classical KTG assumes the interactions (or encounters) between two colliding particles to be elastic and there is no loss of total kinetic energy in the process. This assumption enables us to derive a time-independent velocity distribution function (VDF), i.e., the Maxwell-Boltzmann (MB) velocity distribution function which is given by,

\[ f_{\text{MB}}(\vec{v}, t) = \left( \frac{1}{\pi v_0^2} \right)^{d/2} \exp \left( -\frac{v^2}{v_0^2} \right), \quad v_0^2 = \frac{2\langle \vec{v}^2 \rangle}{d}, \]  

\( (2.1) \)
where \( d \) is the dimensionality. Given a gas of elastically colliding particles, the VDF relaxes to the MB form within a few collisions per particle.

Granular Gases are prototype inelastic gases, i.e., a large conglomerate of dissipatively interacting spheres sufficiently dilute so that the interval of interaction is small compared to the time of flight and the physical dimensions of spheres are small compared to the mean free path, the average distance between successive collisions [4]. The particles are modelled as hard spheres with instantaneous collisions, or as viscoelastic spherical particles with a finite time of contact [5]. This allows for a small deformation on and around the point of contact. The core of the interacting potential is still very strongly repulsive so that the time of contact is very small. To introduce dissipation a non-conservative viscous force is added.

It is evident that the VDF for granular gases is time-dependent as both the total energy and average velocity have an explicit dependence on time. To account for inelastic interactions, the concepts of kinetic theory need to be revisited. The plan of this chapter is as follows. In Sec. 2.2, we define the distribution functions and describe their properties and formulate the problem of kinetic theory. Section 2.3 deals with the inelastic version of the BE equation. We derive the time-dependence of an arbitrary physical quantity \( \langle \psi(t) \rangle \) in Sec. 2.4. In Sec. 2.5 we discuss the Sonine polynomial expansion method to solve the BE equation, and obtain an expression for the first nontrivial expansion coefficient.
2.2 The Velocity Distribution Function

Given a gas of $N$ identical classical particles and its initial condition, i.e., the particle positions $\{r_i(0)\}_{i=1}^{N}$ and velocities $\{v_i(0)\}_{i=1}^{N}$, the configuration at a later time can be found by solving the corresponding Newton’s equations. To extract macroscopic information from the microscopic information of such a system, however, it is not necessary to integrate the corresponding equations of motion explicitly. Also, the macroscopic properties do not depend on the motion of each individual particle. They depend on average properties or the statistical properties of the system. We define the distribution function $f(\vec{r}, \vec{v}, t)$ such that $f(\vec{r}, \vec{v}, t) \, d\vec{r} \, d\vec{v}$ gives the number of particles in an infinitesimal phase space volume $d\vec{r} \, d\vec{v}$ centered around $(\vec{r}, \vec{v})$, or,

$$dN = f(\vec{r}, \vec{v}, t) \, d\vec{r} \, d\vec{v},$$

with a normalization that there are in all $N$ particles

$$N = \int f(\vec{r}, \vec{v}, t) \, d\vec{r} \, d\vec{v}.$$  

For a homogeneous system, the distribution function is independent of $\vec{r}$. Then, the VDF has the following properties, owing to the relation between various moments of $f(\vec{v}, t)$ and the different macroscopically observed quantities:

$$\int f(\vec{v}, t) \, d\vec{v} = \frac{N}{V} = n,$$  

$$\int \vec{v} f(\vec{v}, t) \, d\vec{v} = n\langle \vec{v} \rangle = 0,$$  

$$\int \frac{1}{2} m v^2 f(\vec{v}, t) \, d\vec{v} = n \left\langle \frac{1}{2} m v^2 \right\rangle = \frac{3}{2} n T(t).$$

The BE equation governs the temporal evolution of the one-particle distribution function in a gas of particles interacting only through binary collisions. The main
difficulty in the solution of the BE equation is due to the collision term which depends on the precise nature of intermolecular forces. While modelling the BE equation, one looks for special intermolecular forces such that the differential scattering cross section or collision rate has a simple dependence on the energies of the colliding particles or on the scattering angle. One may also construct mathematical models, where the collision term is modelled in such a way that on the one hand it becomes amenable to analytical treatment and on the other hand preserves the essential properties of the nonlinear Boltzmann equation, such as conservation laws and H-theorem [3].

2.3 The Boltzmann-Enskog Equation for Inelastic Gases

The system under study here is a collection of smooth inelastic hard discs or spheres \((d = 2, 3)\) [6, 7, 8]. The interaction between two hard spheres is modelled by instantaneous collisions with abrupt change in velocities. The total momentum in an inelastic collision between two particles \(i, j\) having masses given by \(m_i, m_j\) remains conserved, hence we have

\[
m_i \vec{v}_i' + m_j \vec{v}_j' = m_i \vec{v}_i + m_j \vec{v}_j. \tag{2.7}
\]

Here, \(\vec{v}_i, \vec{v}_j\) refer to the pre-collision velocities; and \(\vec{v}_i', \vec{v}_j'\) are the post-collision velocities. The normal component of the relative velocity is diminished in the inelastic collision by a factor \(e\) as shown in Fig. 2.1, i.e.,

\[
(\vec{v}_i' - \vec{v}_j') \cdot \hat{n} = - e (\vec{v}_i - \vec{v}_j) \cdot \hat{n}. \tag{2.8}
\]
Elastic Collision

\[(v'_j \cdot v'_2)_n = (v_2 - v_j)_n\]

Inelastic Collision

\[(v'_j \cdot v'_2)_n = e (v_2 \cdot v_j)_n\]

where \(0 < e < 1\)

Figure 2.1: Elastic and inelastic collisions.
Here $e$, the coefficient of restitution, assumes values between 0 and 1 depending on the amount of inelasticity; and $\hat{n}$ is a unit vector pointing from the centre of particle $j$ to $i$. Combining Eqs. (2.7) and (2.8), we obtain

$$
\vec{v}_i' \cdot \hat{n} = \left( \frac{m_i - em_j}{m_i + m_j} \right) \vec{v}_i \cdot \hat{n} + \left( \frac{m_j}{m_i + m_j} \right) (1 + e) \vec{v}_j \cdot \hat{n},
$$

$$
\vec{v}_j' \cdot \hat{n} = \left( \frac{m_j - em_i}{m_i + m_j} \right) \vec{v}_j \cdot \hat{n} + \left( \frac{m_i}{m_i + m_j} \right) (1 + e) \vec{v}_i \cdot \hat{n}.
$$

(2.9)

The parallel component of velocity remains the same.

For the special case where $m_i = m_j = m$, we obtain the following collision rules,

$$
\vec{v}_i' = \vec{v}_i - \frac{1 + e}{2} [(\vec{v}_i - \vec{v}_j) \cdot \hat{n}] \hat{n},
$$

$$
\vec{v}_j' = \vec{v}_j + \frac{1 + e}{2} [(\vec{v}_i - \vec{v}_j) \cdot \hat{n}] \hat{n}.
$$

(2.10)

The loss of energy is the difference in kinetic energies before and after the collision. The final energy is given by,

$$
\frac{1}{2} m (\vec{v}_i'^2 + \vec{v}_j'^2) = \frac{1}{2} m \left[ \vec{v}_i^2 + \vec{v}_j^2 - (1 + e) \vec{v}_{ij} \cdot \hat{n} \left\{ \vec{v}_{ij} \cdot \hat{n} - \frac{(1 + e)}{2} \vec{v}_{ij} \cdot \hat{n} \right\} \right],
$$

(2.11)

where $\vec{v}_{ij} = \vec{v}_i - \vec{v}_j$. Whence, we get

$$
\Delta E = \frac{1}{2} m (\vec{v}_i'^2 + \vec{v}_j'^2) - \frac{1}{2} m (\vec{v}_i^2 + \vec{v}_j^2) = -\frac{1}{4} m e (\vec{v}_{ij} \cdot \hat{n})^2,
$$

where $\epsilon = 1 - e^2$ is the dissipation parameter. The restituting (precollision) velocities $(\vec{v}_i'', \vec{v}_j'')$, yielding post collision velocities $(\vec{v}_i, \vec{v}_j)$ are obtained by inverting the above Eqs. (2.10),

$$
\vec{v}_i'' = \vec{v}_i - \frac{1 + e}{2e} [(\vec{v}_i - \vec{v}_j) \cdot \hat{n}] \hat{n},
$$

$$
\vec{v}_j'' = \vec{v}_j + \frac{1 + e}{2e} [(\vec{v}_i - \vec{v}_j) \cdot \hat{n}] \hat{n}.
$$

(2.13)
Let $f(\vec{r}, \vec{v}, t)$ represent the normalized distribution of velocities. For the homogeneous density distribution and assuming molecular chaos, it is independent of position variables and obeys the following BE equation [2, 5],

$$\frac{\partial f(\vec{v}_1, t)}{\partial t} = \chi \sigma^{d-1} \int d\vec{v}_2 \int d\hat{n} \left( \vec{v}_{12} \cdot \hat{n} \right) \left\{ \frac{1}{\epsilon^2} f(\vec{v}_1', t) f(\vec{v}_2'', t) - f(\vec{v}_1, t) f(\vec{v}_2, t) \right\}$$

$$= \chi \sigma^{d-1} I(f, f),$$

(2.14)

where $\sigma$, $d$ are the particle diameter and dimension respectively, $\vec{v}_{12} = \vec{v}_1 - \vec{v}_2$ and $\chi(n)$ is the pair correlation function at contact for hard spheres with density $n$. Further, $I(f, f)$ is called the collision integral and is given by,

$$I(f, f) = \chi \sigma^{d-1} \int d\vec{v}_2 \int d\hat{n} \left( \vec{v}_{12} \cdot \hat{n} \right) \left\{ \frac{1}{\epsilon^2} f(\vec{v}_1', t) f(\vec{v}_2'', t) - f(\vec{v}_1, t) f(\vec{v}_2, t) \right\}.$$

(2.15)

The prime over the integration in Eqs. (2.14) and (2.15) denotes the restriction $\vec{v}_{12} \cdot \hat{n} > 0$ on the integral, i.e., we consider only the particles that move towards each other.

The factor $(1/\epsilon^2)$ in the gain term originates from the Jacobian

$$d\vec{v}_1'' d\vec{v}_2'' = (1/\epsilon) \ d\vec{v}_1 d\vec{v}_2,$$

(2.16)

and from the length of the collision cylinder.

We assume here that the system of inelastic particles passes through a sequence of equilibrium states, similar to an adiabatic cooling process. It is quite obvious that the VDF is time-dependent as both the average speed and temperature are decreasing with time. It has been argued, though, that the scaled distribution profile may preserve form. The following scaling ansatz has been suggested by Goldstein and Shapiro [7] and by Esipov and Pöschel [9].

$$f(\vec{v}, t) = \frac{1}{v_0^d(t)} \tilde{f}(\tilde{c}),$$

(2.17)

27
where $\bar{c} = \bar{\nu}/v_0(t)$. The time-dependent scaling parameter $v_0(t)$ is related to the temperature, and temperature is related to the second moment of the VDF in the following manner,

$$T(t) = \frac{1}{2} v_0^2(t) = \frac{1}{d} \int d\bar{v} \ v^2 \ f(\bar{v}, t).$$

(2.18)

The time dependence of temperature is given by.

$$\frac{dT}{dt} = \frac{1}{d} \int d\bar{v}_1 \ v_1^2 \ \frac{\partial f(\bar{v}_1, t)}{\partial t} = \frac{\chi \sigma^{d-1}}{d} \int d\bar{v}_1 \ v_1^2 \ I(f, f).$$

(2.19)

Inserting the scaling ansatz in the collision integral $I(f, f)$, we may get a relation between $I(f, f)$ and the dimensionless collision integral $\hat{I}(\hat{f}, \hat{f})$ in the following manner,

$$I(f, f) = \int d\bar{v}_2 \int d\hat{n} \ (\bar{v}_{12} \cdot \hat{n}) \ \left\{ \frac{1}{e^2} f(\bar{v}_1'', t) f(\bar{v}_2'', t) - f(\bar{v}_1, t) f(\bar{v}_2, t) \right\}$$

$$= v_0^d v_0 v_0^{-2d} \int d\bar{c}_2 \int d\hat{n} \ (\bar{c}_{12} \cdot \hat{n}) \ \left\{ \frac{1}{e^2} f(\bar{c}_1'', t) f(\bar{c}_2'', t) - f(\bar{c}_1, t) f(\bar{c}_2, t) \right\}$$

$$= \frac{v_0}{v_0} \hat{I}(\hat{f}, \hat{f}),$$

(2.20)

where we have used the relation $d\bar{\nu} = v_0^d \ d\bar{c}$. The factors $v_0$ and $v_0^{-2d}$ respectively arise from the length of the collision cylinder and from the product of the two distribution functions in the gain and loss terms.

The negative of the moments of the dimensionless collision integral $\hat{I}(\hat{f}, \hat{f})$ are particularly useful in this case as they contain the information about the dissipation, and are defined in the following way,

$$\mu_k = -\int d\bar{c} \ c^k \ \hat{I}(\hat{f}, \hat{f}).$$

(2.21)

Inserting Eqs. (2.18) and (2.20) in Eq. (2.19), we obtain the following equation for the time-dependence of temperature,

$$\frac{dT}{dt} = \frac{\chi \sigma^{d-1}}{d} \left( v_0^2 c_1^2 \right) \left( v_0^d \ d\bar{c}_1 \right) \left( \frac{v_0}{v_0^d} \right) \ \hat{I}(\hat{f}, \hat{f}).$$

(2.22)
Using the definition of the moments of the dimensionless collision integral from Eq. (2.21), we can write Eq. (2.22) in the following way,

$$\frac{dT}{dt} = \frac{\chi \sigma^{d-1} v_0^3}{d} \int c_1^2 d\vec{c}_1 \hat{I}(\hat{r}, \hat{f}) = -\frac{\mu_2}{d} \chi \sigma^{d-1} v_0^3.$$  \hspace{1cm} (2.23)

The Enskog collision frequency for elastic hard spheres is defined as,

$$\omega_0 = \frac{\chi \sigma^{d-1}}{\sqrt{2\pi}} \left( \int d\hat{n} (\hat{v}_{12} \cdot \hat{n}) \right)_0 = \frac{\Omega_d}{\sqrt{2\pi}} \chi \sigma^{d-1} v_0,$$  \hspace{1cm} (2.24)

Here $\langle \ldots \rangle_0$ denotes the average over MB velocity distributions for $\vec{v}_1$ and $\vec{v}_2$ at temperature $T = \frac{1}{2} mv_0^2$ and $\Omega_d = (2\pi^{d/2}) \Gamma(d/2)$ is the surface area of a $d$-dimensional hypersphere of unit radius. Equation (2.23) then becomes,

$$\frac{dT}{dt} = -2\gamma \omega_0 T,$$  \hspace{1cm} (2.25)

where

$$\gamma = (\sqrt{2\pi}/\Omega_d) \frac{\mu_2}{d}$$  \hspace{1cm} (2.26)

is the time-independent dimensionless cooling rate. The average collision per particle is often used as an alternative unit of time which is defined as $d\tau = \omega(T(t)) \ dt$. Integrating we get the following relations for the time dependence of temperature,

$$T(t) = \frac{T_0}{(1 + \gamma t/t_0)^2}; \quad T(\tau) = T_0 \exp(-2\gamma \tau),$$  \hspace{1cm} (2.27)

where we have used the relation $\omega(T) \sim T^{1/2}$. For small inelasticity and in the initial cooling regime, the distribution function can be approximated by the scaled ME distribution $\phi(c)$, i.e.,

$$\hat{f}(c) \sim \phi(c) = \pi^{-d/2} \exp(-c^2)$$  \hspace{1cm} (2.28)
Substituting \( \phi(c) \) in Eq. (2.21), we can get the value of \( \mu_2 \) and the cooling rate 
\[ \gamma_0 = \epsilon/2d, \]
where \( \epsilon = 1 - e^2 \) is the dissipation parameter. Inserting \( \gamma_0 \) in Eq. (2.27) 
we get the Haff's cooling law [10],
\[ T(t) = \frac{T_0}{(1 + t/t_0)^2}, \quad T(\tau) = T_0 \exp(-\epsilon \tau/d). \]  

The time-independent equation for the scaled VDF \( \dot{f}(\tilde{c}) \) is found by inserting the scaling ansatz (2.17) in the BE equation (2.14),
\[ \text{LHS} = \frac{\partial f(\tilde{v}_1, t)}{\partial t} = \frac{\partial}{\partial t} \left( \frac{1}{v_0^d(t)} \dot{f}(\tilde{c}) \right) \]

\[ = \left( -\frac{d}{v_0^{d+1}} \dot{f}(\tilde{c}_1) + \frac{1}{v_0^d} \frac{\partial \dot{f}(\tilde{c}_1)}{\partial c_1} \frac{\partial c_1}{\partial v_0} \right) \frac{dv_0}{dt} \]

\[ = \frac{1}{v_0^{d+2}} \left( d\dot{f}(\tilde{c}_1) + c_1 \frac{\partial \dot{f}(\tilde{c}_1)}{\partial c_1} \right) \frac{dT}{dt} \]

\[ = \frac{v_0}{v_0^d} \frac{\mu_2 \chi \sigma^{d-1}}{d} \left( d\dot{f}(\tilde{c}_1) + c_1 \frac{\partial \dot{f}(\tilde{c}_1)}{\partial c_1} \right), \]  

(2.30)

where we have used the relations
\[ \frac{dc}{dv_0} = -\frac{c}{v_0} \quad \text{and} \quad \frac{dv_0}{dt} = \frac{1}{v_0} \frac{dT}{dt} \]  

(2.31)

and the relation between \( \mu_2 \) and the time derivative of temperature given in Eq. (2.23).

The RHS transforms accordingly to,
\[ \text{RHS} = \chi \sigma^{d-1} \dot{I}(f, \dot{f}) = \chi \sigma^{d-1} \frac{v_0}{v_0^d} \dot{I}(\dot{f}, \dot{\dot{f}}), \]  

(2.32)

whence we get the desired relation for the scaled VDF, i.e.,
\[ \frac{\mu_2}{d} \left( d\dot{f}(\tilde{c}_1) + c_1 \frac{\partial \dot{f}(\tilde{c}_1)}{\partial c_1} \right) = \dot{I}(\dot{f}, \dot{\dot{f}}). \]  

(2.33)
2.4 Time-Dependence of $\langle \psi(t) \rangle$

We often need to calculate the time-derivative of a physical quantity $\psi(t)$, e.g., $\psi(t) = v^2$. It is useful to derive the following property of the collision integral. The time derivative of the expectation value of any property $\psi(t)$ is given by,

$$\frac{d}{dt} \langle \psi(t) \rangle = \int dv_1 \psi(v_1) \frac{\partial}{\partial t} f(v_1, t)$$

$$= \chi \sigma^{d-1} \int dv_1 \psi(v_1) I(f, f) = \chi \sigma^{d-1} Q(f, f). \quad (2.34)$$

We can rewrite the above integral as,

$$Q(f, f) = \int dv_1 \psi(v_1) I(f, f)$$

$$= \int dv_1 \int dv_2 \int d\hat{n} (\vec{v}_1 \cdot \hat{n}) \int' d\hat{n} (\vec{v}_2 \cdot \hat{n}) f(v_1) f(v_2) \psi(v_1)$$

$$- \int dv_1 \int dv_2 \int' d\hat{n} (\vec{v}_1 \cdot \hat{n}) f(v_1) f(v_2) \psi(v_1)$$

$$= Q_1 - Q_2. \quad (2.35)$$

Using the relation

$$(1/e^2) |\vec{u}_{12} \cdot \hat{n}| dv_1 dv_2 = |\vec{u}_{12}'' \cdot \hat{n}| dv_1'' dv_2'' , \quad (2.36)$$

and interchanging $\{ (\vec{v}_1'', \vec{v}_2''), (\vec{u}_1, \vec{u}_2) \}$ with $\{ (\vec{v}_1', \vec{v}_2'), (\vec{v}_1', \vec{v}_2') \}$ in the first integral, we get,

$$Q_1 = \frac{1}{2} \int dv_1 \int dv_2 \int d\hat{n} (\vec{v}_1 \cdot \hat{n}) f(v_1) f(v_2) \{ \psi(v_1') + \psi(v_2') \}. \quad (2.37)$$

Here we have invoked the symmetry between exchange of indices $1 \leftrightarrow 2$. The second term can similarly be manipulated to give,

$$Q_2 = \frac{1}{2} \int dv_1 \int dv_2 \int d\hat{n} (\vec{v}_1 \cdot \hat{n}) f(v_1) f(v_2) \{ \psi(v_1') + \psi(v_2') \}. \quad (2.38)$$
Hence, the time derivative of \( \langle \psi(t) \rangle \) is given by,

\[
\frac{d}{dt} \langle \psi(t) \rangle = \frac{\chi^{d-1}}{2} \int d\vec{v}_1 \int d\vec{v}_2 \int d\vec{n} \, (\vec{v}_{12} \cdot \hat{n}) f(\vec{v}_1) f(\vec{v}_2) \Delta \{ \psi(\vec{v}_1) + \psi(\vec{v}_2) \}. \tag{2.39}
\]

Similarly, it can be shown that in terms of scaled quantities,

\[
\int d\vec{c}_1 \psi(\vec{c}_1) \hat{f}(\hat{f}, \hat{f}) = \frac{1}{2} \int d\vec{c}_1 \int d\vec{c}_2 \int d\hat{n} \, (\vec{c}_{12} \cdot \hat{n}) f(\vec{c}_1) f(\vec{c}_2) \Delta \{ \psi(\vec{c}_1) + \psi(\vec{c}_2) \}. \quad \tag{2.40}
\]

In particular, choosing \( \psi(c) = e^{\beta} \) we get the values of \( \mu_2 \) taken with a negative sign,

\[
\mu_2 = -\frac{1}{2} \int d\vec{c}_1 \int d\vec{c}_2 \int d\hat{n} \, (\vec{c}_{12} \cdot \hat{n}) f(\vec{c}_1) f(\vec{c}_2) \{ \Delta c_1^2 + \Delta c_2^2 \}. \quad \tag{2.41}
\]

### 2.5 Sonine Polynomial Expansion

The initial distribution profile of the velocity of an inelastic gas deviates from the MB distribution. In the limiting case of vanishing dissipation the solution, however, approaches the MB distribution. This suggests the expansion of \( \hat{f}(c) \) about \( \phi(c) \) in terms of some polynomials \( S_p \),

\[
\hat{f}(c) = \phi(c) \left( 1 + \sum_{p=1}^{\infty} a_p S_p(c) \right). \tag{2.42}
\]

We choose \( S_p \) to be the Sonine polynomials, which are nothing but the Associated Laguerre polynomials, and are given as follows [11, 12],

\[
S_p(x) = \sum_{m=0}^{p} (-1)^m x^m \frac{(p - 1 + \frac{d}{2})!}{(p - m)! m! (m - 1 + \frac{d}{2})!}. \tag{2.43}
\]

The first few Sonine polynomials are as follows,

\[
S_0(x) = 1, \tag{2.44}
\]

\[
S_1(x) = \frac{d}{2} - x, \tag{2.45}
\]

\[
S_2(x) = \frac{d(d+2)}{8} - \frac{(d+2)}{2} x + \frac{x^2}{2}, \tag{2.46}
\]

\[
S_3(x) = \frac{d(d+2)(d+4)}{48} - \frac{(d+2)(d+4)}{8} x + \frac{(d+4)}{4} x^2 - \frac{x^3}{6}. \tag{2.47}
\]
\[ S_4(x) = \frac{d(d+2)(d+4)(d+6)}{384} - \frac{(d+2)(d+4)(d+6)}{12} x^3 + \frac{x^4}{24} \]  
\[ (2.48) \]
\[ S_5(x) = \frac{d(d+2)(d+4)(d+6)(d+8)}{3840} \frac{1}{(d+4)(d+6)} x^2 - \frac{(d+2)(d+4)(d+6)(d+8)}{48} x^3 + \frac{d(d+2)(d+4)(d+6)(d+8)}{3840} \]  
\[ (2.49) \]

Choosing \( x = c^2 \) after rearranging terms, we obtain the even powers of \( c \) in terms of these polynomials, i.e.,

\[ c^0 = 1 = S_0(c^2), \]
\[ c^2 = \frac{d}{2} - S_1(c^2), \]
\[ c^4 = \frac{d(d+2)}{4} - (d+2)S_1(c^2) + 2S_2(c^2). \]  
\[ (2.50) \]

We use the following normalization condition:

\[ \int_0^\infty dc \, \phi(c) S_m(c^2) S_n(c^2) = \delta_{nm} \frac{\Gamma(n + d/2)}{n! \Gamma(d/2)} = \delta_{nm} N_n. \]  
\[ (2.51) \]

The first few normalization constants are,

\[ N_0 = 1, \]  
\[ (2.52) \]
\[ N_1 = d/2, \]  
\[ (2.53) \]
\[ N_2 = d(d+2)/8. \]  
\[ (2.54) \]

The above Eqs. (2.50) are used to calculate the moments of the distribution functions.

\[ \langle c^n \rangle = \int c^n \, f(c) \, dc. \]  
\[ (2.55) \]
For example,

\[ \langle c^2 \rangle = \int d\bar{c} \, c^2 \left( \frac{d}{2} - S_1 \right) \phi(c) \left( 1 + \sum_{i=1}^{\infty} a_i S_i \right) \]

\[ = \int d\bar{c} \, \phi(c) \left( S_0 + \sum_{i=1}^{\infty} a_i S_i \right) \left( \frac{d}{2} S_0 - S_1 \right) \]

\[ = (1 - a_1) \frac{d}{2}. \tag{2.56} \]

Hence we have,

\[ a_1 = 0, \tag{2.57} \]

where we have used the orthogonality relations Eq. (2.51) and \( \langle c^2 \rangle = d/2 \) by the definition of temperature. Equation (2.57) is general and significant in the sense that it tells us that the first deviations from the MB distribution starts from \( a_2 \). Similarly,

\[ \langle c^4 \rangle = (1 + a_2) \frac{d(d+2)}{4}. \tag{2.58} \]

For the moments \( \mu_p \) we combine Eqs. (2.21) and (2.33) to obtain

\[ \mu_p = - \int d\bar{c} \, c^p \hat{f} = - \int d\bar{c} \, c^p \left( \frac{\mu_2}{d} \right) \left( d + c \frac{d}{dc} \right) \hat{f}(c) \]

\[ = -\mu_2 \langle c^p \rangle \frac{\mu_2}{d} \int_0^{\infty} d\bar{c} \, c^{p+1} \frac{df}{dc} \]

\[ = -\mu_2 \langle c^p \rangle - \frac{\mu_2}{d} \int_0^{\infty} \Omega_d \, c^{p+d} \, df. \tag{2.59} \]

Partially integrating the above, and assuming that \( \hat{f}(c) \) decays faster than any power of \( c \) (and hence \( c^{p+d} \hat{f}(c) \to 0 \) as \( c \to \infty \)), we obtain,

\[ \mu_p = -\mu_2 \langle c^p \rangle + \frac{\mu_2}{d} (p + d) \langle c^p \rangle = \frac{\mu_2}{d} p \langle c^p \rangle. \tag{2.60} \]

In principle all the coefficients of the scaling function \( \hat{f}(c) = \phi(c)(1 + \sum a_n S_n) \) can be calculated. The process, however, becomes very cumbersome even for the first
nontrivial coefficient $a_2$. If we assume that the major contribution to the deviation arises from $a_2$, then we can restrict the series to $f(c) = \phi(c)(1 + a_2 S_2)$. Equation (2.41) then can be rewritten in the form.

\[
\mu_p = -\frac{1}{2} \int d\tilde{c}_1' d\tilde{c}_2' \int' d\tilde{n} \, (\tilde{c}_{12} \cdot \tilde{n}) \, \phi(c_1) \, \phi(c_2) \\
\times [1 + a_2 \{ S_2(c_1^2) + S_2(c_2^2) \} + a_2^2 S_2(c_1^2) S_2(c_2^2)] \, [\Delta c_p^2 + \Delta c_p^2].
\]  

(2.61)

To evaluate the above expression, it is convenient to use the relative and centre of mass velocities, defined as,

\[
\tilde{c}_1 = \tilde{C} + \frac{1}{2} \tilde{c}_{12} \quad ; \quad \tilde{c}_1 = \tilde{C} - \frac{1}{2} \tilde{c}_{12}.
\]

(2.62)

It can easily be verified that the Jacobian of the transformation is unity. The other quantities transform as follows.

\[
\phi(c_1) \, \phi(c_2) = \pi^{-d} \exp(-c_1^2) \exp(-c_2^2) \\
= \left\{ (2\pi)^{-d/2} \exp\left(-\frac{1}{2} \tilde{c}_{12}^2\right) \right\} \{(\pi/2)^{-d/2} \exp(-2C^2)\}
\]

(2.63)

The term in the braces transforms to,

\[
\{ S_2(c_1^2) + S_2(c_2^2) \} = \frac{d(d+2)}{4} - \frac{(d+2)}{2} (c_1^4 + c_2^4) + \frac{1}{2} (c_1^4 + c_2^2)
\]

\[
= \frac{d(d+2)}{4} - (d+2) \left(C^4 + \frac{c_{12}^2}{4}\right) + C^4 + \frac{1}{16} c_{12}^4 + \frac{1}{2} C^2 c_{12}^2 (\tilde{C} \cdot \tilde{c}_{12})^2.
\]

(2.64)

Finally, in order to calculate $\Delta c_p^{\alpha}$ we write the collision rules in terms of the relative and centre of mass velocities, i.e.,

\[
\tilde{c}_1' = \tilde{C} + \frac{1}{2} \tilde{c}_{12} - \frac{1}{2} (1 + e) \, (\tilde{c}_{12} \cdot \tilde{n}) \, \tilde{n},
\]

(2.65)

\[
\tilde{c}_2' = \tilde{C} - \frac{1}{2} \tilde{c}_{12} + \frac{1}{2} (1 + e) \, (\tilde{c}_{12} \cdot \tilde{n}) \, \tilde{n}.
\]

(2.66)

35
whence it is easy to get the following expressions.

$$\Delta (c_1^2 + c_2^2) = -\frac{1 - e^2}{2} (\vec{c}_{12} \cdot \hat{n})^2. \quad (2.67)$$

$$\Delta (c_1^4 + c_2^4) = 2(1 + e)^2 (\vec{c}_{12} \cdot \hat{n})^2 (\vec{C} \cdot \hat{n})^2 + \frac{1}{8} (1 - e^2)^2 (\vec{c}_{12} \cdot \hat{n})^4$$

$$- \frac{1}{4} (1 - e^2) (\vec{c}_{12} \cdot \hat{n})^2 \vec{c}_{12}^2 - (1 - e^2) \vec{C}^2 (\vec{c}_{12} \cdot \hat{n})^2$$

$$- 4(1 + e)(\vec{C} \cdot \vec{c}_{12}) (\vec{C} \cdot \hat{n}) (\vec{c}_{12} \cdot \hat{n}). \quad (2.68)$$

In order to proceed further, we need the solution of the integrals of the following type,

$$J_{k,l,m,n,p,a} = \int d\vec{c}_{12} d\vec{C} \int d\hat{n} (\vec{c}_{12} \cdot \hat{n})^{1+\alpha} \phi(c_{12}) \phi(C)$$

$$C^{k} c_{12}^{l} (\vec{C} \cdot \vec{c}_{12})^{m} (\vec{C} \cdot \hat{n})^{n} (\vec{c}_{12} \cdot \hat{n})^{p}. \quad (2.69)$$

We give here the general solution of Eq. (2.69) in $d$-dimensions for $n = 0, 1, 2$. (For the proof of the solution one may refer to [5]).

$$J_{k,l,m,n,p,a} = (-1)^p [1 + (-1)^m] 2^{l+m+p+\alpha+1} \Omega_d^{-1}$$

$$\times \beta_{p+\alpha+1} \beta_{m} \gamma_{k+m+n+m+p+\alpha+1}, \quad (2.70)$$

$$J_{k,l,m,1,p,a} = (-1)^{p+1} [1 + (-1)^{m+1}] 2^{l+m+p+\alpha+1} \Omega_d^{-1}$$

$$\times \beta_{p+\alpha+2} \beta_{m+1} \gamma_{k+m+1+n+m+p+\alpha+1}, \quad (2.71)$$

$$J_{k,l,m,2,p,a} = (-1)^p [1 + (-1)^m] 2^{l+m+p+\alpha+1} [(d-1) \Omega_d]^{-1}$$

$$\times \gamma_{k+m+2} \gamma_{l+m+p+\alpha+1} [(d \beta_{p+\alpha+3} - \beta_{p+\alpha+1}) \beta_{m+2}$$

$$+(\beta_{p+\alpha+1} - \beta_{p+\alpha+3}) \beta_{m}], \quad (2.72)$$

where $\Omega_d = \frac{2 \pi^{d/2}}{\Gamma\left(\frac{d}{2}\right)}$ is the surface area of a $d$-dimensional unit sphere and the other
quantities are given as follows,

\[ \beta_m = \int' d\hat{n} \ (\hat{c}_{12} \cdot \hat{n})^m \]
\[ = \frac{1}{2} \Omega_d \int' d\hat{n} \ (\cos \theta)^m \]
\[ = \frac{1}{2} \Omega_d \int_0^{\pi/2} d\theta (\sin \theta)^{d-2} (\cos \theta)^m \]
\[ = \pi^{(d-1)/2} \frac{\Gamma(m+1)}{\Gamma(m+d)} \] \quad (2.73)

\[ \gamma_r = \int d\hat{C} C^r \phi(C) \]
\[ = \int_0^\infty C^{d-1+r} \left( \frac{2}{\pi} \right)^{d/2} \exp(-2C^2) dC \int d\hat{C} \]
\[ = \left( \frac{2}{\pi} \right)^{d/2} \frac{1}{4} \frac{\sqrt{2} \Gamma \left( \frac{d+r}{2} \right)}{\sqrt{2}^{d+r-1} \Omega_d} \gamma_r \]
\[ = 2^{-(r/2)} \frac{\Gamma \left( \frac{d+r}{2} \right)}{\Gamma \left( \frac{d}{2} \right)} \] \quad (2.74)

With the help of Eqs. (2.64), (2.67) and (2.68), we can reduce \( \mu_2 \) to the following form,

\[ \mu_2 = \frac{1}{4} (1 - e^2) \left\{ J_{0,0,0,0,2,0} + a_2 \left( J_{4,0,0,0,2,0} + J_{0,0,2,0,2,0} + \frac{1}{16} J_{0,4,0,0,2,0} + \frac{1}{2} J_{2,2,0,0,2,0} \right) - (d + 2) J_{2,0,0,0,0,2,0} - \frac{(d + 2)}{4} J_{2,0,0,0,0,2,0} + \frac{d(d + 2)}{4} J_{0,0,0,0,2,0} \right\} \] \quad (2.75)

Inserting the values of various \( J_{k,l,m,n,p,o} \) in Eq. (2.75) we get

\[ \mu_2 = \frac{1}{2} (1 - e^2) \frac{\Omega_d}{\sqrt{2\pi}} \left\{ 1 + \frac{3}{16} a_2 \right\} \] \quad (2.76)

Similarly we can find out the value of \( \mu_4 \)

\[ \mu_4 = \frac{\Omega_d}{\sqrt{2\pi}} \{ T_1 + a_2 T_2 \} \] \quad (2.77)

37
where.

\[ T_1 = \frac{1}{4}(1 - e^2)(d + \frac{3}{2} + e^2), \tag{2.78} \]
\[ T_2 = \frac{3}{128}(1 - e^2)(10d + 39 + 10e^2) + \frac{1}{4}(1 + e)(d - 1). \tag{2.79} \]

From Eqs. (2.76), (2.77) and (2.58), we know the values of \( \mu_2, \mu_4 \) and \( \langle c^4 \rangle \). Introducing them in Eq. (2.60) Noije and Ernst (NE) [6] obtained a closed equation for \( a_2 \) which can be solved. Hence we obtain

\[ a_2^{NE} = \frac{16(1 - e)(1 - 2e^2)}{9 + 24d + 8de - 41e + 30(1 - e)e^2}. \tag{2.80} \]

One can extend the series to \( \hat{f}(c) = \phi(c)(1 + a_2S_2 + a_3S_3) \) or even to higher order.

The calculation, however, increases in complexity to an extent that manually it is difficult to calculate them. Using a Maple program Brilliantov and Pöschel (BP) [1, 13, 14] have calculated \( a_2 \) and \( a_3 \) using a more sophisticated expansion than NE [6]. The BP calculation accounts for the influence of \( a_3 \), which is assumed to be negligible in the NE study. They obtain the following expressions in \( d = 2 \) [13]:

\[
\begin{align*}
a_2 &= -\frac{16}{b(e)}(-849 + 1170e - 291e^2 + 708e^3 + 2782e^4 - 6400e^5 \\
&\quad + 3120e^6 - 480e^7 + 240e^8), \tag{2.81}
\end{align*}
\]

\[
\begin{align*}
a_3 &= -\frac{128}{b(e)}(183 - 342e - 543e^2 + 1340e^3 + 66e^4 - 1344e^5 \\
&\quad + 720e^6 - 160e^7 + 80e^8), \tag{2.82}
\end{align*}
\]

\[
\begin{align*}
b(e) &= 102195 - 128358e + 70017e^2 + 9060e^3 + 15950e^4 - 74240e^5 \\
&\quad + 34800e^6 - 5600e^7 + 2800e^8. \tag{2.83}
\end{align*}
\]

38
The corresponding $d = 3$ results are [14]

$$a_2 = \frac{16}{c(e)} (-1623 + 1934e + 895e^2 - 364e^3 + 3510e^4 - 7424e^5 
+ 3312e^6 - 430e^7 + 240e^8), \tag{2.84}$$

$$a_3 = \frac{128}{c(e)} (217 - 386e - 669e^2 + 1548e^3 + 154e^4 - 1600e^5
+ 816e^6 - 160e^7 + 80e^8), \tag{2.85}$$

$$c(e) = 214357 - 172458e + 112155e^2 + 25716e^3 - 4410e^4 - 84480e^5
+ 34800e^6 - 5600e^7 + 2800e^8. \tag{2.86}$$

We will compare our MD data presented in Chapter 3 with the results obtained by NE and BP. In Fig. 2.2(a), we plot $a_2$ and $a_3$ vs. $e$ for $d = 2$ and $e \in [0, 1]$. We compute $a_2$ using the NE result in Eq. (2.80) (solid line) and the BP result in Eq. (2.81) (dashed line). Our MD results in Chapter 3 are obtained for $e \in [0.7, 1]$. For these values of $e$, there is little difference between $a_2^{NE}$ and $a_2^{BP}$. Further, the typical values of $a_3$ are 4-5 times smaller than the corresponding $a_2$. Figure 2.2(b) is the 3-d counterpart of Fig. 2.2(a).
Figure 2.2: (a) Plot of analytical expressions for $a_2$ and $a_3$ in $d = 2$. For $a_2$, we show the Noije-Ernst (NE) result in Eq. (2.80) [6]; and the Brilliantov-Poschel (BP) result in Eq. (2.81) [13]. For $a_3$, we show the BP result in Eq. (2.82) [13]. (b) Analogous to (a) but for $d = 3$. We plot the NE result for $a_2$ in Eq. (2.80); the BP result for $a_2$ in Eq. (2.84) [14]; and the BP result for $a_3$ in Eq. (2.85) [14].
Bibliography


