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Lattice Boltzmann Method for Bosons and Fermions

Rodrigo Carlos Viana Coelho

Dissertação de Mestrado apresentada ao Programa de Pós-Graduação em Física do Instituto de Física da Universidade Federal do Rio de Janeiro - UFRJ, como parte dos requisitos necessários à obtenção do título de Mestre em Ciências (Física).

Orientador: Mauro Melchiades Doria

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1. Introduction. 2. Hydrodynamics and conservations laws. 3. The Lattice Boltzmann Method. 4. The quantum fluid. 5. Applications of the quantum hydrodynamics. 6. Numerical results. 7. Conclusion. A. Hermite polynomials. B. Chapmann-Enskog assumption and the conservation laws. C. Gauss-Hermite quadrature. D. Useful relations.

Resumo

O Método Lattice-Boltzmann Aplicado a Bósons and Férmions

Rodrigo Carlos Viana Coelho

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Resumo da Dissertação de Mestrado apresentada ao Programa de Pós-Graduação em Física do Instituto de Física da Universidade Federal do Rio de Janeiro - UFRJ, como parte dos requisitos necessários à obtenção do título de Mestre em Ciências (Física).

Nos anos 80, foi desenvolvido um método numérico para a resolução da equação de Boltzmann com o termo de colisão de Bhatnagar, Gross e Krook (BGK). Este método, baseado na discretização do espaço de posição e velocidade, teve grande sucesso na resolução de vários problemas de escoamento de fluidos[1]. Conhecido como LBM (*Lattice Bolztmann Method*), o método do reticulado de Boltzmann descreve a evolução temporal de um conjunto de distribuições estatísticas de partículas definidas numa rede espacial regular, na qual cada sítio possui um número finito de velocidades direcionadas para os sítios vizinhos. Na simplicidade de sua dinâmica e principalmente na flexibilidade para a implementação computacional de maneira paralela, reside a sua vantagem sobre outros métodos. O LBM leva às equações hidrodinâmicas do continuo na escala macroscópica, tais como as de conservação de massa e de momento (Navier Stokes). Nos últimos anos tem sido feito um grande esforço para a construção de um LBM capaz de descrever fluidos compressíveis e térmicos, o que acarreta também na descrição do transporte de energia.

[1]Ver: http://www.palabos.org/

Nesta dissertação desenvolvo o LBM para o tratamento dos fluidos quânticos, ou seja, aqueles tais que as distribuições de partículas descrevem bósons ou férmions. Mostro que o LBM do fluido clássico térmico e compressível, descrito pela estatística de Maxwell-Boltzmann, e o LBM do fluido quântico, descrito pelas estatísticas de Fermi-Dirac e Bose-Einstein, se assentam na mesma estrutura matemática. Ambos os casos exigem a expansão até quarta ordem das funções de distribuição de equilíbrio em polinômios de Hermite, de tal forma que as equações hidrodinâmicas possuem uma termodinâmica consistente. Desta feita obtenho as equações macroscópicas que descrevem o fluido quântico, isto é, a equação de conservação de massa, momento (Navier-Sokes) e a equação da conservação da energia. Resultam destas equações os coeficientes de viscosidade e condutividade térmica conhecidos. Como aplicação do LBM obtido, faço simulações numéricas para partículas quânticas diluídas com condições de contorno periódicas e considero diferentes condições iniciais.

Key-words: LBM térmico, fluido quântico, expansão em polinômios de Hermite, mecânica estatística.

Abstract

Lattice Boltzmann Method for Bosons and Fermions

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Abstract da Dissertação de Mestrado apresentada ao Programa de Pós-Graduação em Física do Instituto de Física da Universidade Federal do Rio de Janeiro - UFRJ, como parte dos requisitos necessários à obtenção do título de Mestre em Ciências (Física).

In the 80s a numerical method was developed to solve the Boltzmann equation with the BGK (Bhatnagar, Gross and Krook) collision term. This method, based on the discretization of the phase space, was very successful in solving various problems of fluid mechanics, including problems with complex geometry, interfacial phenomena and multicomponent fluids [28]. Known as the LBM – Lattice Bolztmann Method – it describes the evolution of a set of statistical distributions of particles defined on a regular space lattice in which each site has a finite number of velocities directed to neighbouring sites. The advantage over other methods lies in the simplicity of its dynamics and especially the flexibility for implementation in parallel computing. The LBM leads to the expected hydrodynamic equations in the continuous macroscopic scale, such as conservation of mass and momentum (Navier Stokes). In recent years there has been a great interest in the construction of an LBM able to describe compressible and thermal fluids, which also carries the description of energy conservation [21].

In this thesis we develop the LBM for the treatment of quantum fluids, i.e., those such that the statistical distribution of particles describe bosons or fermions. We show

that the LBM for the thermal and compressible classical fluid, described by the Maxwell-Boltzmann statistics, and the LBM for the quantum fluids, described by the Bose-Einstein and Fermi-Dirac statistics, are based on the same mathematical structure. Both cases require the expansion to fourth order of the equilibrium distribution functions in Hermite polynomials to obtain macroscopic hydrodynamical equations consistent with thermodynamics. Therefore we show in this thesis that only in case this expansion is carried to fourth order the correct macroscopic equations describing the quantum fluid are obtained, i.e., the equations for the conservation of mass, momentum (Navier-Sokes) and energy. From these equations we retrieve the well-known coefficients of viscosity and thermal conductivity. As an application, we do numerical simulations for diluted quantum particles with periodic boundary conditions considering different initial conditions.

Keywords: Thermal LBM, quantum fluid, Hermite polynomials expansion, statistical mechanics.

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Chapter 1

Introduction

One of the greatest achievements of the Boltzmann equation [14] is to determine the macroscopic hydrodynamical equations of a fluid from a phase space distribution function, $f(\boldsymbol{\chi}, \boldsymbol{x}, t)$, which describes the probability to find particles with microscopic velocity $\boldsymbol{\chi}$ in position $\boldsymbol{x}$ at time t. Nearly eighty years have passed since E. A. Uehling and G. E. Uhlenbeck [37] solved the Boltzmann equation for the quantum fluid approximately by determining the small correction to the distribution function of non-interacting particles in case of a weak interaction. From this solution they derived the macroscopic hydrodynamical equations through the so-called Chapman-Enskog analysis and obtained the viscosity, η, and the thermal conductivity, κ, coefficients of the quantum fluid. The Uehling-Uhlenbeck approach was later revisited by T. Nikuni and A. Griffin [22] who derived the macroscopic hydrodynamic equations, and the corresponding η and κ coefficients, of a trapped Bose gas above the Bose-Einstein condensation with damping. C. H. Lepienski and G. M. Kremer [16] also determined these coefficients in case of specific two-body potentials, namely, Lennard-Jones and hard spheres. Recently the Boltzmann equation was found applicable to describe the collective oscillations of the two-dimensional Fermi gas [39]. All the above studies of the quantum fluid take the assumption of a two-body collision operator, as in the original Bolztmann equation. A simplifying assumption for the collision operator was introduced in the fifties by Bhatnagar-Gross-Krook (BGK) [4], who considered it just as a simple drive to an *equilibrium distribution function* under a single relaxation time

τ. Nevertheless only recently the Uehling-Uhlenbeck approach was applied to solve the BGK-Boltzman equation for the quantum fluid [32, 42] by J.Y. Yang et al., who derived its η and κ coefficients.

In the late eighties a numerical scheme was formulated to solve the Boltzmann equation with the BGK collision term [19, 35, 36, 41] under the assumption of a discrete phase space where both the microscopic velocity and the position are restricted to a discrete set of values defined by a lattice. This method became widely known as the lattice Boltzmann method (LBM) and is used to simulate fluids with numerous advantages, such as easy implementation, inherent parallelization, and flexible treatment of the boundary conditions. The position space falls on a regular lattice where each point has a discrete set of microscopic velocity vectors that points towards a selected set of nearest nodes. To this discrete set of directions we associate the index α, such that the microscopic velocities become $\boldsymbol{\chi}_\alpha$. The neighbor points are reached after a time Δt. The discreteness and rigidity of the microscopic velocity in the LBM makes the distribution function also become a discrete set, and instead of $f(\boldsymbol{\chi}, \boldsymbol{x}, t)$, one has $f_\alpha(\boldsymbol{x}, t)$, fact that is of great numerical advantage. Then the lattice BGK-Boltzmann equation is derived from the continuous Boltzmann equation under a discretization procedure [11],

$$f_\alpha(\boldsymbol{x} + \boldsymbol{\chi}_\alpha \Delta t, t + \Delta t) - f_\alpha(\boldsymbol{x}, t) = -\frac{\Delta t}{\tau}\left[f_\alpha(\boldsymbol{x}, t) - f_\alpha^{(0)}(\boldsymbol{x}, t)\right], \tag{1.1}$$

which constantly drives the non-equilibrium distribution $f_\alpha(\boldsymbol{x}, t)$ to the equilibrium distribution function $f_\alpha^{(0)}(\boldsymbol{x}, t)$. Despite the tremendous success of the LBM method to describe the mass and momentum (Navier-Stokes) equations, the inclusion of a energy equation remained a challenge for sometime. The energy equation is needed to describe, for instance, the conversion of friction due to motion into heat, that increases the fluid temperature. This means that the transport of matter by particle diffusion is intertwined with the advected transport of enthalpy in such a way that the total energy is conserved for a closed system. The macroscopic hydrodynamical equations of the classical thermal compressible

fluid are well-known, and can be derived from general macroscopic principles, as shown in the book of Landau & Lifshitz [15], for instance.

Many years after the development of the Uehling-Uhlenbeck approach, H. Grad [9,18] devised another method to solve the continuous Boltzmann equation based on a sequence of approximations, obtained through the expansion of the distribution function in terms of the microscopic velocity space, expressed as a gaussian times a linear expansion in Hermite polynomials. Grad's approach turned to be of paramount importance for the understanding of the properties of the LBM. For this reason the Hermite polynomial expansion method found a renewal of interest, such as in Refs. [30, 31]. Despite the understanding brought by these references, the ingredients to describe the thermal compressible classical fluid were still missing, since the Hermite polynomial expansion was only carried there until third order ($N = 3$), which is just insufficient. It was not until recently that the LBM for the thermal compressible fluid with a single BGK relaxation time, as described in Eq.(1.1), was derived. Philippi et al. (Ref. [24]), Siebert et al. (Ref. [34]), and Shan and Chen (Ref. [29]), succeeded to show that the thermal compressible properties of the classical fluid are correctly described if the Hermite polynomial expansion is carried until fourth order ($N = 4$). Then the Chapman-Enskog analysis [24, 29, 34], applied to the BGK-Boltzmann equation with the Maxwell-Boltzmann equilibrium distribution function, gives the macroscopic hydrodynamical equations for the mass, momentum and energy balance, as obtained in the book of Landau & Lifshitz [15].

This master's thesis is organized as follows. In chapter 2, we review the classical macroscopic hydrodynamical equations as described by Landau & Lifshitz [15] and, in the end of this chapter, introduce the results that will be obtained by Chapman-Enskog analysis. The chapter 3 is also a review, where we present some basic concepts necessary to understand the LBM. There is a original content in this chapter, section 3.2, that is the expansion of the MB distribution function by Taylor series until fourth order in macroscopic velocity $\boldsymbol{u}$. The chapter 4 we derive the major result of this thesis, which is

a consistent LBM for quantum fluids. We obtain the expansion in Hermite polynomials of the BE and FD distributions until fourth order, get the correct macroscopic equations for the quantum fluid by Chapman Enskog analysis and discuss several of their aspects, such as the introduction of the pseudo variables and the viscosity and thermal coefficients. In section 4.5 we obtain a no go theorem for the Hermite polynomial expansion to order $N = 3$. In chapter 5, we apply the macroscopic equations for quantum fluids obtained in the previous chapter to a few situations already known from the classical hydrodynamics. The chapter 6 shows the numerical simulations with the dilute quantum fluid and the classical fluid. In appendix A, we present the Hermite polynomials. Appendix B shows that the Chapman-Enskog assumption is necessary to get the conservation laws of mass, momentum and energy. In appendix C we see the Gauss-Hermite quadrature and some examples of lattices in one, two and three dimensions and, finally, in appendix D, there are some relations that are useful to perform the Chapman Enskog analysis.

There has been in the past years attempts to construct a LBM for the classical thermal compressible fluid starting from *ad hoc* assumptions of the equilibrium distribution function [2, 6, 10, 25, 26, 41]. This approach was never attempted for the quantum fluid.

Chapter 2

Hydrodynamics and conservations laws

In this chapter we review the macroscopic equations that govern the compressible thermal fluid. These equations can be derived from general thermodynamic principles and Newton's laws applied to continuum media. Here we shall follow closely the derivation of such equations as done by Landau and Lifshitz [15]. Newton´s laws determines the motion of atoms and molecules, the microscopic particles that comprise the fluid, whose average motion defines the motion of the fluid. A fundamental concept in the study of fluids is the so-called element of a fluid or fluid particle. The element of a fluid takes an infinitesimal volume that contains many microscopic particles, thus its size is larger than the inter-atomic distance and yet much smaller than the macroscopic dimensions.

The fluids, unlike the solids, don't have a well defined volume. If we put, for example, a liquid or a gas in a container, it would acquire the shape of the recipient.

Nevertheless we define an *element of fluid* or *fluid particle*, which has an infinitesimal volume with many microscopic particles and still is much smaller than the macroscopic dimensions. The element of a fluid can be thought as being in the mesoscopic scale. Once understood the concept of this element the fluid can be considered as a continuous media. Then naturally arises two ways to study the fluid dynamics: the Lagrangian and the Eulerian description of fluid flow. In the Lagrangian description, one seeks to

determine the individual trajectories of the elements of fluid as they move along and together establish the macroscopic fluid flow. Thus the goal is to determine the trajectory and velocity of enach element of fluid as a function of time. In the Eulerian description, we fix an element in space in position $\mathbf{x} = \hat{\mathbf{x}}x + \hat{\mathbf{y}}y + \hat{\mathbf{z}}z$ and study the fluid moving through this point. We shall follow here the Eulerian approach to obtain the macroscopic equations of the compressible thermal flow.

Thus to correctly describe a moving fluid we must determine five variables in each element of fluid, namely, the three components of the velocity (in 3-dimensional space), $\boldsymbol{v}(\mathbf{x})$ and also two thermodynamic quantities that belongs to fluid among the three existing ones, namely the pressure $p(\mathbf{x})$, the density $\rho(\mathbf{x})$, and the temperature $T(\mathbf{x})$. This is because we accept that these three variables satisfy a constitutive equation, for example, the law of perfect gases, $p/\rho T = const.$.

Next we seek to determine the conservations laws that are fundamental to determine the fluid dynamics.

The conservation of matter leads to the so-called *continuity equation*. Given a volume V_0 in space, the total mass inside this volume (figure 2.1) is the integral of the density times the volume,

$$m = \int_{V_0} \rho \, d^3r, . \tag{2.1}$$

The flux of fluid that flows through an infinitesimal area $\hat{\mathbf{n}}d^2r$, where $\hat{\mathbf{n}}$ is the normal vector pointing outward the surface is $\rho\boldsymbol{u} \cdot \hat{\mathbf{n}}d^2r$. So, the total flux through the surface of V_0 is

$$\oint_{\partial V_0} \rho\boldsymbol{u} \cdot \hat{\mathbf{n}}d^2r. \tag{2.2}$$

We calculate the variation of mass in V_0 in two ways: by deriving (2.1) or by (2.2). Equationg the both ways

$$-\frac{\partial}{\partial t}\int \rho d^3r = \oint \rho\boldsymbol{u} \cdot \hat{\mathbf{n}}d^2r,$$

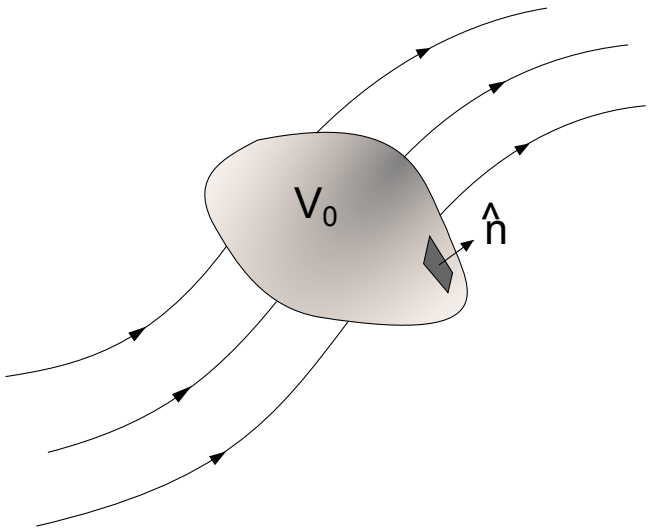

Figure 2.1: Volume V_0 of space inside the fluid. The normal vector $\hat{\mathbf{n}}$ points outwards

but we can use the divergence theorem to transform the surface integral

$$\oint_{\partial V_0} \rho \boldsymbol{u} \cdot \hat{\mathbf{n}} d^2 r = \int_{V_0} \nabla \cdot (\rho \boldsymbol{u}) d^3 r.$$

Thus,

$$\int_{V_0} \left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) \right] d^3 r = 0.$$

Since the integral must hold for any volume in the fluid, the equation in the brackets is zero

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0. \tag{2.3}$$

This is the so-called *continuity equation*, which is a general statement applicable to both ideal and viscous fluid. The discussion of the conservation of momentum and and energy must take into account whether the fluid is ideal or not. For this reason we firstly consider the ideal fluid.

2.1 Ideal Flows

In ideal fluids the energy does not dissipate. There is no internal friction (viscosity) between fluid particles nor heat exchange between different parts of the fluid. The last

imposition also includes the assumption that the fluid doesn't exchange heat with the boundaries what means the ideal fluid must be adiabatic.

2.1.1 Euler's equation

The total force acting in a volume of the fluid is

$$\mathbf{F} = \mathbf{F}_{ext} - \oint p\,\hat{\mathbf{n}}\,d^2r = \mathbf{F}_{ext} - \int \nabla p\,d^3r,$$

where the divergence theorem was used. Force by unity of volume is $\mathbf{f} = \mathbf{f}_{ext} - \nabla p$. Writing the second Newton's Law for the fluid

$$\rho\frac{d\boldsymbol{u}}{dt} = \mathbf{f}_{ext} - \nabla p. \tag{2.4}$$

As an example of external force, consider the gravitational interaction that is $\mathbf{f_{ext}} = \nabla(\rho g z)$, where g is the local acceleration of gravity and z is the height of fluid column

$$\rho\frac{d\boldsymbol{u}}{dt} = -\nabla(p - \rho g z).$$

The pressure can be understood as a density of potential energy.

The treatment of the acceleration, $d\boldsymbol{u}/dt$, reveals fundamental distinctions between the Lagrangian and Eulerian approaches to fluids. As the acceleration is also fundamental to formulate Newton's third law for fluids, this treatment must be carefully discussed. The time derivative denotes a change in the velocity of a fluid while it moves in space in the Lagrangian description. Since $\boldsymbol{u}[x(t), y(t), z(t), t]$, this means that $\frac{d}{dt} \equiv \frac{\partial}{\partial t} + \frac{\partial}{\partial x(t)}\frac{dx(t)}{dt} + \frac{\partial}{\partial y(t)}\frac{dy(t)}{dt} + \frac{\partial}{\partial z(t)}\frac{dz(t)}{dt}$. It happens that in the Eulerian description, x, y, z, and u_x, u_y and u_z are all independent variables, and so,

$$\frac{d\boldsymbol{u}}{dt} = \frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u}.$$

Substituting in (2.4), we obtain the *Euler's equation*

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -\frac{1}{\rho}\nabla p + \mathbf{f}_{ext}. \tag{2.5}$$

In summary, the equation of motion for fluids is a direct consequence of Newton's Laws. This equations was obtained by Leonhard Euler and its validity is limited to negligible viscosity and heat conduction. If we consider the external force as being the gravity, we have $\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\frac{1}{\rho}\nabla p + g$.

2.1.2 Momentum flux

Newton's law for fluids can be casted in a different way. Consider again a volume element, which has the momentum $\rho\boldsymbol{u}$. Let us calculate the time variation of momentum in index notation

$$\frac{\partial}{\partial t}(\rho u^i) = \rho\frac{\partial u^i}{\partial t} + \frac{\partial \rho}{\partial t}u^i. \tag{2.6}$$

Using the continuity equation and Euler's equation

$$\begin{aligned}\frac{\partial}{\partial t}(\rho u^i) &= -\rho u^k\frac{\partial u^i}{\partial x^k} - \frac{\partial p}{\partial x^i} - u^i\frac{\partial}{\partial x^k}(\rho u^k) \\ &= -\frac{\partial p}{\partial x^i} - \frac{\partial}{\partial x^k}(\rho u^i u^k) \\ &= -\frac{\partial p}{\partial x^k}\delta^{ik} - \frac{\partial}{\partial x^k}(\rho u^i u^k)\end{aligned} \tag{2.7}$$

and defining the *momentum flux density tensor* Π^{ik} as

$$\Pi^{ik} = p\delta^{ik} + \rho u^i u^k \tag{2.8}$$

we have that the equation of momentum flux is

$$\frac{\partial}{\partial t}(\rho u^i) = -\frac{\partial}{\partial x^k}\Pi^{ik}. \tag{2.9}$$

2.1.3 Energy flux

The energy stored in some *element of fluid* fixed in space, is the sum of the kinetic energy and internal energy, ε,

$$\frac{1}{2}\rho\boldsymbol{u}^2 + \rho\varepsilon, \tag{2.10}$$

Consider how this stored energy varies with time,

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho\boldsymbol{u}^2 + \rho\varepsilon\right). \tag{2.11}$$

To calculate this time derivative, consider that,

$$\frac{1}{2}\frac{\partial}{\partial t}(\rho \boldsymbol{u}^2) = \frac{1}{2}\boldsymbol{u}^2\frac{\partial \rho}{\partial t} + \rho \boldsymbol{u}\cdot\frac{\partial \boldsymbol{u}}{\partial t}. \tag{2.12}$$

Using the continuity equation and Euler's equation, under the assumption of no external force, $\mathbf{f_{ext}} = 0$, gives that,

$$\frac{1}{2}\frac{\partial}{\partial t}(\rho \boldsymbol{u}^2) = -\frac{1}{2}\boldsymbol{u}^2\nabla\cdot(\rho \boldsymbol{u}) - \boldsymbol{u}\cdot\nabla p - \rho \boldsymbol{u}\cdot[(\boldsymbol{u}\cdot\nabla)\boldsymbol{u}]. \tag{2.13}$$

The gradient of the pressure is dealt by the first law of thermodynamics,

$$d\varpi = Tds + Vdp \Rightarrow \nabla p = \rho\nabla\varpi - \rho T\nabla s, \tag{2.14}$$

where ϖ is the heat function per unit mass (or enthalpy per unity mass, $\varpi = \varepsilon + \frac{p}{\rho}$), s is the entropy per unity mass and V is the volume per unity mass. Using also $\boldsymbol{u}\cdot[(\boldsymbol{u}\cdot\nabla)]\boldsymbol{u} = \frac{1}{2}\boldsymbol{u}\cdot\nabla\boldsymbol{u}^2$, we obtain,

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho\boldsymbol{u}^2\right) = -\frac{1}{2}\boldsymbol{u}^2\nabla\cdot(\rho\boldsymbol{u}) - \rho\boldsymbol{u}\cdot\nabla\left(\frac{1}{2}\boldsymbol{u}^2 + \varpi\right) + \rho T\boldsymbol{u}\cdot\nabla s. \tag{2.15}$$

The above equation is the first term of Eq.(2.11) and it remains to calculate its second term. Using again the first law of thermodynamics and that $V = 1/\rho$, $d\varepsilon = Tds - pdV = Tds + \frac{p}{\rho^2}d\rho$. Notice that $\varepsilon + \frac{p}{\rho} = \varepsilon + pV$ is the heat function per unity mass,

$$\begin{aligned} d(\rho\varepsilon) &= \varepsilon d\rho + \rho d\varepsilon \\ &= \varepsilon d\rho + \rho T ds - \frac{\rho p}{\rho^2}d\rho \\ &= \left(\varepsilon - \frac{p}{\rho}\right)d\rho + \rho T ds \\ &= \varpi\, d\rho + \rho\, T\, ds. \end{aligned} \tag{2.16}$$

Thus, using continuity equation

$$\frac{\partial}{\partial t}(\rho\varepsilon) = \varpi\frac{\partial\rho}{\partial t} + \rho T\frac{\partial s}{\partial t} = -\varpi\nabla\cdot(\rho\boldsymbol{u}) + \rho T\frac{\partial s}{\partial t}. \tag{2.17}$$

Considering a adiabatic transport, which the entropy of the volume element remains constant while the fluid particle moves in space

$$\frac{ds}{dt} = \frac{\partial s}{\partial t} + \boldsymbol{u} \cdot \nabla s = 0 \tag{2.18}$$

or, using the continuity equation

$$\frac{\partial}{\partial t}(\rho s) + \nabla \cdot (\rho s \boldsymbol{u}) = 0, \tag{2.19}$$

that is the *equation for entropy*. Substituting (2.18) in (2.17)

$$\frac{\partial}{\partial t}(\rho\varepsilon) = -\varpi \nabla \cdot (\rho \boldsymbol{u}) - \rho T \boldsymbol{u} \cdot \nabla s. \tag{2.20}$$

Summing (2.15) and (2.20)

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho \boldsymbol{u}^2 + \rho\varepsilon\right) = -\left(\frac{1}{2}\boldsymbol{u}^2 + \varpi\right)\nabla \cdot (\rho \boldsymbol{u}^2) - \rho \boldsymbol{u} \cdot \nabla\left(\frac{1}{2}\boldsymbol{u}^2 + \varpi\right)$$

we finally obtain

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho \boldsymbol{u}^2 + \rho\varepsilon\right) = -\nabla \cdot \left[\rho \boldsymbol{u}\left(\frac{1}{2}\boldsymbol{u}^2 + \varpi\right)\right]. \tag{2.21}$$

The vector $\rho \boldsymbol{u}\left(\frac{1}{2}\boldsymbol{u}^2 + \varpi\right)$ is called the *energy flux density*.

2.2 Equations of motion of a viscous fluid

Fluids are distinct from solids in their resistance to tangential stress. A solid submitted to tangential stress will deform until creates internal stress that balances the external force and remains in equilibrium. If the force is not too large, the solid returns to its initial shape. When we apply tangential stress to a fluid, it flows and the deformation is permanent. With a small force is possible to cause a large deformation in a fluid if we spend enough time. The real fluids offers some resistance to slip adjacent layers due to the exchange of momentum between the layers and that resistance measure the viscosity.

Thus in a viscous fluid, there is friction between adjacent fluid layers and part of the kinetic energy is transformed into thermal energy. This effect cause the thermodynamic irreversibility of the process which is a consequence of the second law of thermodynamics.

2.2.1 Equation of momentum

The basic assumption to derive the equation of momentum flux for viscuous fluids is that the equation (2.9) still holds. Nevertheless to, account for the irreversibility, we have to add the new term $-\sigma'^{ik}$, called *viscosity stress tensor*, to the momentum flux density tensor, which becomes,

$$\Pi^{ik} = p\delta^{ik} + \rho u^i u^k - \sigma'^{ik} = -\sigma^{ik} + \rho u^i u^k, \tag{2.22}$$

where the *stress tensor* has been defined as,

$$\sigma^{ik} = -p\delta^{ik} + \sigma'^{ik}. \tag{2.23}$$

Based on the assumption that the viscosity stress tensor is a sole function of the velocity and only first order derivatives are significant, its general form must be,

$$\sigma'^{ik} = \eta\left(\frac{\partial u^i}{\partial x^k} + \frac{\partial u^k}{\partial x^i} - \frac{2}{3}\delta^{ik}\frac{\partial u^l}{\partial x^l}\right) + \zeta\delta^{ik}\frac{\partial u^l}{\partial x^l}, \tag{2.24}$$

where ζ and η are known as the *volumetric* and *dynamic viscosities* and are non-negative quantities. Summing $\partial\sigma'^{ik}/\partial x^k$ to the right hand of Euler's equation

$$\rho\left(\frac{\partial u^i}{\partial t} + u^k\frac{\partial u^i}{\partial x^k}\right) = -\frac{\partial p}{\partial x^i} + \frac{\partial \sigma'^{ik}}{\partial x^k}$$

or, using the continuity equation,

$$\frac{\partial(\rho u^i)}{\partial t} + \frac{\partial}{\partial x^k}(p\delta^{ik} + \rho u^i u^k - \sigma'^{ik}) = 0. \tag{2.25}$$

This is the general form of the equation of motion for the viscous fluid. In general, ζ and η depend on the temperature and the pressure, thus they are position dependent. Thus, they can't be taken outside the derivative. Next we derive the well-known Navier-Stokes equation for incompressible fluids which assumes that ζ and η are constants:

$$\frac{\partial\sigma'^{ik}}{\partial x^k} = \eta\left(\frac{\partial^2 u^i}{\partial x^k\partial x^k} + \frac{\partial u^k}{\partial x^i\partial x^k} - \frac{2}{3}\frac{\partial^2 u^l}{\partial x^i\partial x^l}\right) + \zeta\frac{\partial^2 u^l}{\partial x^i\partial x^l}. \tag{2.26}$$

The equation of motion becomes,

$$\rho\left(\frac{\partial u^i}{\partial t}+u^k\frac{\partial u^i}{\partial x^k}\right)=-\frac{\partial p}{\partial x^i}+\eta\frac{\partial^2 u^i}{\partial x^k\partial x^k}+\left(\zeta+\frac{\eta}{3}\right)\frac{\partial^2 u^k}{\partial x^i\partial x^k} \tag{2.27}$$

since the fluid is incompressible, $\nabla\cdot\boldsymbol{u}=0$, and the last term vanishes

$$\frac{\partial u^i}{\partial t}+u^k\frac{\partial u^i}{\partial x^k}=-\frac{1}{\rho}\frac{\partial p}{\partial x^i}+\frac{\eta}{\rho}\frac{\partial^2 u^i}{\partial x^k\partial x^k}. \tag{2.28}$$

This is the Navier-Stokes equation for incompressible fluids.

2.2.2 Equation of heat transfer

The study of ideal fluids is the search for mathematical solutions of the continuity equation (Eq.(2.3)), the Euler's equation (Eq.(2.5)) and the conservation of entropy (Eq.(2.18)). They form a complete system of five equations and there are five quantities to determine, the density, the three velocity components and one thermodynamical potential such as the internal energy, since the other ones must be related to this one for an adiabatic flow. For the study of viscous fluids the continuity equation still holds, the Euler's equation is replaced by the Navier-Stokes equation (Eq.(2.25)), and now we can no longer seek the conservation of entropy because the process is irreversible. So we must find another equation to treat the energy, that goes beyond Eq.(2.21):

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho\boldsymbol{u}^2+\rho\varepsilon\right)=-\nabla\cdot\left[\rho\boldsymbol{u}\left(\frac{1}{2}\boldsymbol{u}^2+\varpi\right)\right].$$

As the conservation of energy must still hold in the general case, the only difference is that it must allow for the conversion of mechanical motion into heat, which is also a form of energy. Nevertheless we shall not deal with situation that energy evades away from the system, through other processes not described here, such as the emission of radiation. For such reasons we add irreversibility into the system simply by adding extra terms to the divergence. The term $\boldsymbol{u}\cdot\boldsymbol{\sigma'}$, that is, $u^i\sigma'^{ik}$ in index notation, to account for the convection (with macroscopic transport of fluid) and the term responsible for the conduction of heat (without transport of mass), $-\kappa\nabla T$, that is present even if the fluid is at rest. The

constant κ is known as the *thermal conductivity*. This constant too is assumed positive and can depend on the temperature and the pressure. So, the *general equation of energy conservation* is

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho\boldsymbol{u}^2+\rho\varepsilon\right)=-\nabla\cdot\left[\rho\boldsymbol{u}\left(\frac{1}{2}\boldsymbol{u}^2+\varpi\right)-\boldsymbol{u}\cdot\boldsymbol{\sigma'}-\kappa\nabla T\right]. \tag{2.29}$$

This equations does not treat the heat flux by others sources, as irradiation, but we can add a new term ϕ inside the brackets to account the irradiation. Thus we have also reached five equations to govern the viscous fluid, which is also compressible and thermal.

2.2.3 Overview of macroscopic equations

We establish contact between the above macroscopic hydrodynamical equations and those derived from the Boltzmann equation by firstly casting equations (2.3), (2.25) and (2.29) in a more general form, that will be valid in arbitrary D dimensions for the quantum case [42], which is discussed in chapter 4:

$$\frac{\partial\rho}{\partial t}+\frac{\partial(\rho u^i)}{\partial x^i}=0, \tag{2.30}$$

$$\rho\left(\frac{\partial}{\partial t}+u^i\frac{\partial}{\partial x^j}\right)u^j+\frac{\partial}{\partial x^j}P^{ij}=0, \text{ and} \tag{2.31}$$

$$\frac{\partial}{\partial t}\left(\frac{D}{2}\rho\theta\right)+\frac{\partial}{\partial x^j}\left(\frac{D}{2}\rho\theta u^j\right)+\frac{1}{2}\left(\frac{\partial u^i}{\partial x^j}+\frac{\partial u^j}{\partial x^i}\right)P^{ij}+\frac{\partial Q^i}{\partial x^i}=0. \tag{2.32}$$

These equations are expressed in terms of the stress tensor, P^{ij}, and the heat flux vector, Q^i, that acquire different form, depending whether the quantum or classical fluid is being treated. From the macroscopic thermodynamical derivation of the present chapter, these tensors are,

$$P^{ij}=\rho\theta\delta^{ij}-\sigma^{ij}, \tag{2.33}$$

and

$$Q^i=-\kappa\frac{\partial\theta}{\partial x^i}, \tag{2.34}$$

where, for D dimensions,

$$\sigma^{ij} = \eta \left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i} - \frac{2}{D} \delta^{ij} \frac{\partial u^l}{\partial x^l} \right) + \zeta \delta^{ij} \frac{\partial u^l}{\partial x^l}. \tag{2.35}$$

We shall derive in the this thesis the macroscopic hydrodynamical equations, Eqs.(2.30), (2.31) and (2.32), so far obtained by general macroscopic principles, from the Boltzmann equation. For the classical fluid this results from an Hermite polynomial expansion of the Maxwell-Boltzmann equilibrium distribution function carried until $N = 4$ order [24,29,34], and the subsequent Chapman-Enskog analysis applied to the BGK-Boltzmann equation. However the coefficients acquire special features, such as the viscosity stress tensor has a null volumetric viscosity ($\zeta = 0$), and the dynamic viscosity is given by,

$$\eta \equiv \rho \theta \tau \left(1 - \frac{\Delta t}{2\tau} \right), \tag{2.36}$$

and the thermal conductivity by,

$$\kappa \equiv \left(\frac{D+2}{2} \right) \rho \theta \tau \left(1 - \frac{\Delta t}{2\tau} \right). \tag{2.37}$$

such that $\kappa/\eta = (D+2)/2$. Notice that these coefficients are local because of their θ and ρ dependence. The pressure is $p = \rho\,\theta$, the internal energy is, $\varepsilon \equiv D\theta/2$, such that the enthalpy becomes , $\varpi \equiv (D+2)\theta/2$. The constant τ is a novel physical constant, introduced by the BGK-Boltzmann equation and is a characteristic relaxation time of the system. The constant Δt is a mathematical constant associated to a time step used in the procedure to solve the Boltzmann equation. For the connection to the macroscopic equation the ratio $\Delta t/\tau \ll 1$, and so, can be safely ignored.

Chapter 3

The Lattice Boltzmann Method

3.1 Boltzmann Equation

In this chapter we review the derivation of the Boltzmann equation from basic probabilistic concepts. We derive it in the continuum phase space and also in a discretized one, used to construct the LBM. This chapter also has an original content in the sense that we unveil the mathematical framework that makes possible the construction of the thermal compressible LBM in this discrete phase space.

Consider a monoatomic classical gas of N particles within a volume V at a temperature T in phase space, described by position space, $\mathbf{x}$, and the microscopic velocity space, $\boldsymbol{\chi}$. We introduce the distribution function, $f(\mathbf{x}, \boldsymbol{\chi}, t)$ such that $f(\mathbf{x}, \boldsymbol{\chi}, t)d^3x d^3\chi$ is the number of particles, at time t, in some particular phase space volume, with spatial coordinates and microscopic velocities ranging from $\mathbf{x}$ to $\mathbf{x}+d\mathbf{x}$ and $\boldsymbol{\chi}$ to $\boldsymbol{\chi}+d\boldsymbol{\chi}$, respectively. In case that there is a weak interaction among the particles this function is the *Maxwell-Boltzmann distribution*

$$f^{(0)}(\mathbf{x}, \boldsymbol{\chi}, t) = \rho(\mathbf{x}, t) \left[\frac{m}{2\pi k_B T(\mathbf{x}, t)} \right]^{\frac{D}{2}} e^{-\frac{m[\chi - v(\mathbf{x},t)]^2}{2k_B T(\mathbf{x},t)}} \tag{3.1}$$

where k_B is the Boltzmann's constant, D is the number of spatial dimensions and the index $^{(0)}$ says that we are considering the distribution function as being at equilibrium. We allow the gas density of the ideal gas, $\rho(\mathbf{x})$, the macroscopic velocity, $v(\mathbf{x})$, and the temperature $T(\mathbf{x})$ to be local quantities in position space but not in the microscopic

velocity space. Notice that there is no explicit, and only implicit, dependence of the equilibrium distribution function on $\mathbf{x}$. In fact, these quantities correspond to the first three moments of the above local Maxwell-Boltzmann distribution function obtained by integration over the microscopic velocity $\boldsymbol{\chi}$:

$$\rho(\mathbf{x}) = \int d^D\boldsymbol{\chi}\; f^{(0)}(\boldsymbol{\chi}, \rho, T, \boldsymbol{v}), \tag{3.2}$$

$$\boldsymbol{v}(\mathbf{x}) = \frac{1}{\rho(\mathbf{x})} \int d^D\boldsymbol{\chi}\; \boldsymbol{\chi} f^{(0)}(\boldsymbol{\chi}, \rho, T, \boldsymbol{v}), \tag{3.3}$$

and

$$\frac{D}{2} k_B T(\mathbf{x}) = \frac{1}{\rho(\mathbf{x})} \int d^D\boldsymbol{\chi}\; \frac{1}{2} m \left[\boldsymbol{\chi} - \boldsymbol{v}(\mathbf{x})\right]^2 f^{(0)}(\boldsymbol{\chi}, \rho, T, \boldsymbol{v}). \tag{3.4}$$

From the point of view of the individual particles one expects that a single particle in $(\mathbf{x}, \boldsymbol{\chi})$ at time t moves to $(\mathbf{x} + \boldsymbol{\chi}\Delta t, \boldsymbol{\chi} + (\mathbf{F}/m)\Delta t)$ at time $t + \Delta t$ in phase space, where m is the mass of the particle. We shall take units of $m = 1$ such that the presence of an external force $\mathbf{F}$ becomes acceleration and assume that it is able to change the microscopic velocity $\boldsymbol{\chi}$. We expect this property to be present in the distribution function in phase space, which should be the same at time $t + \Delta t$ and time t in the absence of collisions between particles. But if we consider collisions the distribution functions must change and satisfy the following relation,

$$f(\mathbf{x} + \boldsymbol{\chi}\Delta t, \boldsymbol{\chi} + \mathbf{F}\Delta t, t + \Delta t) = f(\mathbf{x}, \boldsymbol{\chi}, t) + \left(\frac{\partial f}{\partial t}\right)_{coll} \Delta t, \tag{3.5}$$

we can expand the left hand side in Taylor series until first order in Δt

$$f(\mathbf{x}, \boldsymbol{\chi}, t) + \frac{\partial f}{\partial t}\Delta t + \frac{\partial f}{\partial x^i}\chi^i \Delta t + \frac{\partial f}{\partial \chi^i} F^i \Delta t + O[(\Delta t)^2] = f(\mathbf{x}, \boldsymbol{\chi}, t) + \left(\frac{\partial f}{\partial t}\right)_{coll} \Delta t,$$

So

$$\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x^i}\chi^i + \frac{\partial f}{\partial \chi^i} F^i = \left(\frac{\partial f}{\partial t}\right)_{coll}. \tag{3.6}$$

This is the celebrated *Boltzmann equation* in its general form [27]. The terms on the left hand side are the drift terms, and, on the right hand side, we have the collision operator,

where are all information about atomic aspects of scattering process. It is remarkable that from such straightforward statistical concepts, Boltzmann was able to obtained a simple equation which leads to the macroscopic equations of hydrodynamics.

3.1.1 Collision operator for binary collisions

In this section we determine the collision term of Eq.(3.6) under some assumptions [14]: (i) a dilute gas, such that only binary collisions are taken into account; (ii) the force between any two particles is much larger than the external force; (iii) the velocities of any two particles at any time and their respective coordinates are not correlated, and (iv) the distribution function can only vary over a distance comparable to the mean free path[1].

In figure 3.1, we see two rigid spheres of radius $a/2$ colliding elastically with each other, where b is the impact parameter and θ is the scattering angle. The velocities of the particles before the collision are $\boldsymbol{\chi_1}$ and $\boldsymbol{\chi_2}$, so that the relative velocity is $\boldsymbol{\chi} = \boldsymbol{\chi_2} - \boldsymbol{\chi_1}$, and, due to conservation of momentum

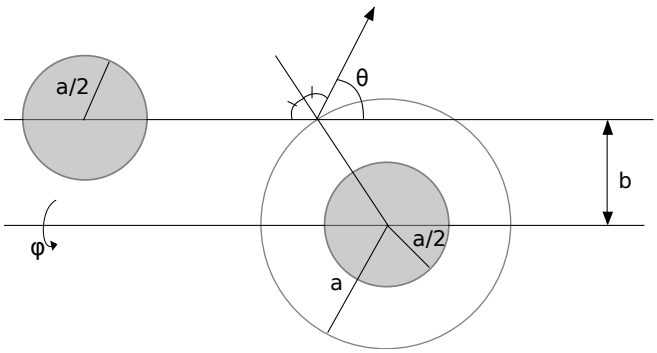

Figure 3.1: Schematic representation of the collision, with impact parameter b and scattering angle θ, between two rigid spheres of diameter a.

$$\boldsymbol{\chi_2} + \boldsymbol{\chi_1} = \boldsymbol{\chi_2'} + \boldsymbol{\chi_1'}, \tag{3.7}$$

being $\boldsymbol{\chi_1'}$ and $\boldsymbol{\chi_2'}$ the velocities after collision. From conservation of energy

$$|\boldsymbol{\chi_2}|^2 + |\boldsymbol{\chi_1}|^2 = |\boldsymbol{\chi_2'}|^2 + |\boldsymbol{\chi_1'}|^2. \tag{3.8}$$

[1]The mean free path is the average distance travelled by a moving particle between two successive collisions with other moving particles. See *http://hyperphysics.phy-astr.gsu.edu/hbase/kinetic/menfre.html* for instance.

Thus, we obtain

$$|\boldsymbol{\chi_2} - \boldsymbol{\chi_1}| = |\boldsymbol{\chi_2'} - \boldsymbol{\chi_1'}|, \tag{3.9}$$

that is, the modulus of relative velocity before ($\boldsymbol{\chi}$) and after ($\boldsymbol{\chi'}$) impact is the same (all particles have the same mass). We may write a collision term for a dilute gas and binary collision as

$$\left(\frac{\partial f}{\partial t}\right)_{coll} \Delta t = (R_f - R_i)\Delta t, \tag{3.10}$$

where $R_i d^3x d^3\chi \Delta t$ is the number of collisions that occur in the interval Δt so that one of initial particles is inside the element volume in phase space $d^3x d^3\chi$ and $R_f d^3x d^3\chi \Delta t$ is the number o collisions between t and $t + \Delta t$ in a way that one of the final particles is within the volume element $d^3x d^3\chi$. The distribution function is independent of position since the system is uniform. The elementary volume of the collision cylinder is given by $(\chi \Delta t)(db)(bd\phi)$ and we can determine $b < a$ so as the collision occur. By the figure 3.1,

$$\sin\left(\frac{\pi - \theta}{2}\right) = \frac{b}{a} \;\Rightarrow\; db = -\frac{a}{2}\sin\frac{\theta}{2}d\theta, \tag{3.11}$$

so, the elementary volume becomes

$$b\,\Delta t\,\chi\,db\,d\phi = \frac{1}{2}a^2\chi\sin\frac{\theta}{2}\cos\frac{\theta}{2}d\theta d\phi\Delta t = \frac{1}{4}a^2\chi\sin\theta d\theta d\phi\Delta t \tag{3.12}$$

Thus

$$R_i\Delta t d^3\chi_1 = \int_{\boldsymbol{\chi_2}}\int_{\Omega}\left[|\boldsymbol{\chi_2} - \boldsymbol{\chi_1}|\frac{a^2}{4}d\Omega\Delta t\right] f(\boldsymbol{\chi_1}, \boldsymbol{\chi_2}, t)d^3\chi_1 d^3\chi_2 \tag{3.13}$$

where $d\Omega = \sin\theta d\theta d\phi$ and $f(\boldsymbol{\chi_1}, \boldsymbol{\chi_2}, t)d^3\chi_1 d^3x_1 d^3\chi_2 d^3x_2$ is the number of pair of particles, at time t, with coordinates in phase space inside $d^3\chi_1 d^3x_1$ and $\chi_2 d^3x_2$ respectively. According to molecular chaos hypothesis

$$f(\boldsymbol{\chi_1}, \boldsymbol{\chi_2}, t) = f(\boldsymbol{\chi_1}, t)f(\boldsymbol{\chi_2}, t). \tag{3.14}$$

The Eq.(3.13) now is

$$R_i\Delta t d^3\chi_1 = \int_{\Omega}\frac{1}{4}a^2 d\Omega\int_{\boldsymbol{\chi_2}}|\boldsymbol{\chi_2} - \boldsymbol{\chi_1}|f(\boldsymbol{\chi_1}, t)f(\boldsymbol{\chi_2}, t)d^3\chi_1 d^3\chi_2 \tag{3.15}$$

The equation for R_f can be obtained considering the reverse collision $(\boldsymbol{\chi_1'};\boldsymbol{\chi_2'}) \rightarrow (\boldsymbol{\chi_1};\boldsymbol{\chi_2})$. Analogously

$$R_f \Delta t d^3\chi_1 = \int_\Omega \frac{1}{4} a^2 d\Omega \int_{\boldsymbol{\chi_2}} |\boldsymbol{\chi_2'} - \boldsymbol{\chi_1'}| f(\boldsymbol{\chi_1'}, t) f(\boldsymbol{\chi_2'}, t) d^3\chi_1' d^3\chi_2', \tag{3.16}$$

using Eq.(3.9) and that $d^3\chi_1 d^3\chi_2 = d^3\chi_1' d^3\chi_2'$ we finally write the collision term

$$\left(\frac{\partial f_1}{\partial t}\right)_{coll} = \int_\Omega \frac{1}{4} a^2 d\Omega \int_{\boldsymbol{\chi_2}} d^3\chi_2 |\boldsymbol{\chi_2} - \boldsymbol{\chi_1}| (f_1' f_2' - f_1 f_2), \tag{3.17}$$

where $f_1 = (\boldsymbol{\chi_1}, t)$, $f_1' = (\boldsymbol{\chi_1}', t)$ and so on. The Boltzmann equation stays [27]

$$\left(\frac{\partial}{\partial t} + \chi^i \frac{\partial}{\partial x^i} + F^i \frac{\partial}{\partial \chi^i}\right) f(\mathbf{x}, \boldsymbol{\chi}, t) = \int_\Omega \sigma(\Omega) d\Omega \int_{\boldsymbol{\chi_2}} d^3\chi_2 |\boldsymbol{\chi_2} - \boldsymbol{\chi_1}| (f_1' f_2' - f_1 f_2) \tag{3.18}$$

with $\sigma(\Omega)$ being a velocity-independent cross section. We can recover the Maxwell-Boltzmann distribution (Eq.(3.1)) by setting null the collision operator in Eq.(3.17) [14].

3.1.2 The BGK collision operator

In this section we discuss another collision operator for Eq.(3.6), which is simpler than the binary one. The Eq.(3.17) is a tricky form of the collision operator because it involves a product of two distribution and the Boltzmann equation becomes a complicated integro-differential equation for determining the non-equilibrium distribution. We show that this simpler collision term is able to preserves the basic physical properties of Eq.(3.17), i.e., conservation of mass, momentum and energy. This is the so-called *BGK operator*

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = -\frac{f - f^{(0)}}{\tau}. \tag{3.19}$$

where τ is the *relaxation time*, and $f^{(0)}$ is the equilibrium distribution, that for classical case reduces to Eq.(3.1). This operator was first proposed by Bhatnagar, Gross, and Krook in 1954 and it assumes that the rate at which f returns to the equilibrium distribution $f^{(0)}$ due to scattering is proportional to the deviation of f from $f^{(0)}$. Thus, the Boltzmann equation with BGK collision operator (from now on we will call it BGK-Boltzmann) is,

$$\left(\frac{\partial}{\partial t} + \chi^i \frac{\partial}{\partial x^i} + F^i \frac{\partial}{\partial \chi^i}\right) f(\mathbf{x}, \boldsymbol{\chi}, t) = -\frac{f - f^{(0)}}{\tau}. \tag{3.20}$$

This equation is much more easier to treat than Eq.(3.18).

Previously we have shown how to derive the continuous Boltzmann equation (Eq. (3.20)) from the discrete form (Eq.(3.5)). Here we show that this can be done in the reverse way and derive the discrete Boltzmann equation from the continuum one [11].

The BGK-Boltzmann equation without external force can be expressed as,

$$\frac{\partial f}{\partial t} + \boldsymbol{\chi} \cdot \nabla f = -\frac{1}{\tau^*}(f - f^{(0)}), \tag{3.21}$$

where τ^* is the dimensional relaxation time due to collision. This equation (3.21) can be rewritten using the convective derivative $d/dt = \partial/\partial t + \boldsymbol{\chi} \cdot \nabla$, that is

$$\frac{df}{dt} + \frac{1}{\tau^*} f = \frac{1}{\tau^*} f^{(0)}. \tag{3.22}$$

This equation can be integrated over a time step of Δt giving

$$f(\boldsymbol{x}+\boldsymbol{\chi}\Delta t, \boldsymbol{\chi}, t+\Delta t) = \frac{1}{\tau^*} e^{-\frac{\Delta t}{\tau^*}} \int_0^{\Delta t} e^{\frac{t'}{\tau^*}} f^{(0)}(\boldsymbol{x}+\boldsymbol{\chi}t', \boldsymbol{\chi}, t+t')dt' + e^{-\frac{\Delta t}{\tau^*}} f(\boldsymbol{x}, \boldsymbol{\chi}, t). \tag{3.23}$$

If we assume that Δt is sufficiently small and $f^{(0)}$ is smooth enough, the following expansion can be made

$$\begin{aligned} & f^{(0)}(\boldsymbol{x} + \boldsymbol{\chi}t', \boldsymbol{\chi}, t + t') \\ & = \left(1 - \frac{t'}{\Delta t}\right) f^{(0)}(\boldsymbol{x}, \boldsymbol{\chi}, t) + \frac{t'}{\Delta t} f^{(0)}(\boldsymbol{x} + \boldsymbol{\chi}\Delta t, \boldsymbol{\chi}, t + \Delta t) + O[(\Delta t)^2] \end{aligned}$$

for $0 \leq t' \leq \Delta t$. Neglecting terms of order $O[(\Delta t)^2]$, Eq.(3.23) stay

$$\begin{aligned} & f(\boldsymbol{x} + \boldsymbol{\chi}\Delta t, \boldsymbol{\chi}, t + \Delta t) - f(\boldsymbol{x}, \boldsymbol{\chi}, t) = (e^{-\frac{\Delta t}{\tau^*}} - 1)[f(\boldsymbol{x}, \boldsymbol{\chi}, t) - f^{(0)}(\boldsymbol{x}, \boldsymbol{\chi}, t)] \\ & + \left[1 + \frac{\tau^*}{\Delta t}(e^{-\frac{\Delta t}{\tau^*}} - 1)\right] [f^{(0)}(\mathbf{x} + \boldsymbol{\chi}\Delta t, \boldsymbol{\chi}, t + \Delta t) - f^{(0)}(\mathbf{x}, \boldsymbol{\chi}, t)]. \end{aligned}$$

Expanding $e^{-\frac{\Delta t}{\tau^*}} \cong 1 - \frac{\Delta t}{\tau^*}$ and defining $\tau \equiv \tau^*/\Delta t$ we finally have

$$f(\boldsymbol{x} + \boldsymbol{\chi}\Delta t, \boldsymbol{\chi}, t + \Delta t) - f(\boldsymbol{x}, \boldsymbol{\chi}, t) = -\frac{1}{\tau}[f(\boldsymbol{x}, \boldsymbol{\chi}, t) - f^{(0)}(\boldsymbol{x}, \boldsymbol{\chi}, t)], \tag{3.24}$$

where τ is a dimensionless relaxation time. Therefore, we made the discretization of time that is represented by the above equation. This is the *lattice Boltzmann equation*, that is a finite-difference form of the continuous Boltzmann equation. This equation simply stems by taking that $df/dt = [f(\boldsymbol{x} + \boldsymbol{\chi}\Delta t, \boldsymbol{\chi}, t + \Delta t) - f(\boldsymbol{x}, \boldsymbol{\chi}, t)]/\Delta t$.

3.1.3 The Chapman-Enskog assumption

In this section we review the so-called Chapman-Enskog assumption which are of fundamental assumptions for the Boltzmann equation theory. Their motivation leads to the derivation of the macroscopic hydrodynamical equations from the Boltzmann equation (see appendix B). Thus thanks to them the mesoscopic world, described by the Boltzmann equation, is linked to the macroscopic world of the hydrodynamical equations.

Basically they correspond to the assumption that the first three macroscopic moments, i.e., the mass density ρ, the macroscopic velocity $\boldsymbol{v}$ and the energy density $\varepsilon = \frac{D}{2}k_B T(\mathbf{x})$ can be either computed from the known equilibrium distribution function $f^{(0)}$ or from the non-equilibrium distribution function f, which satisfies the Boltzmann equation:

$$\rho = \int f d^D\chi = \int f^{(0)} d^D\chi, \tag{3.25}$$

$$\rho\boldsymbol{v} = \int \boldsymbol{\chi} f d^D\chi = \int \boldsymbol{\chi} f^{(0)} d^D\chi, \text{and} \tag{3.26}$$

$$\rho\varepsilon = \frac{1}{2}\int (\boldsymbol{\chi} - \boldsymbol{v})^2 f d^D\chi = \frac{1}{2}\int (\boldsymbol{\chi} - \boldsymbol{v})^2 f^{(0)} d^D\chi. \tag{3.27}$$

In more general grounds the *Chapman-Enskog assumption* can be casted as,

$$\int \psi(\boldsymbol{\chi}) f(\boldsymbol{x}, \boldsymbol{\chi}, t) d^D\chi = \int \psi(\boldsymbol{\chi}) f^{(0)}(\boldsymbol{x}, \boldsymbol{\chi}, t) d^D\chi, \tag{3.28}$$

where $\psi(\boldsymbol{\chi})$ is a linear combination of collisional invariants, that is, conserved quantities

$$\psi(\boldsymbol{\chi}) = A + \mathbf{B}\cdot\boldsymbol{\chi} + C\boldsymbol{\chi}\cdot\boldsymbol{\chi}, \tag{3.29}$$

with A and C being arbitrary scalar constants and $\mathbf{B}$ being an arbitrary constant vector.

3.2 Taylor expansion of the Maxwell-Boltzmann distribution function

In this section we show a remarkable property of the taylor expanded Maxwell-Boltzmann distribution. The three free parameters of the full Maxwell-Boltzmann distribution, namely, the density, macroscopic velocity and temperature, are also present in

the taylor expanded version. Remarkably for the taylor expanded distribution function these three parameters remain as its three first moments, fact that is known to be true for the full Maxwell-Boltzmann distribution. This is the feature that opens the gate for the construction of the LBM, as seen here for the thermal compressible fluid.

Firstly we introduce dimensionless units based on a reference temperature T_r, not present in the original Maxwell-Boltzmann distribution, that also defines a reference velocity:

$$c_r \equiv \sqrt{\frac{k_B T_r}{m}}, \tag{3.30}$$

Then there is dimensionless temperature,

$$\theta \equiv \frac{T}{T_r}, \tag{3.31}$$

and dimensionless microscopic and macroscopic velocities, defined as,

$$\boldsymbol{\xi} \equiv \frac{\boldsymbol{\chi}}{c_r}, \text{ and } \boldsymbol{u} \equiv \frac{\boldsymbol{v}}{c_r}. \tag{3.32}$$

Thus the Maxwell-Boltzmann equilibrium distribution in reduced units becomes,

$$f(\boldsymbol{\xi}) \equiv \rho \left(\frac{1}{2\pi\theta}\right)^{\frac{D}{2}} e^{-\frac{(\boldsymbol{\xi}-\boldsymbol{u})^2}{2\theta}}, \tag{3.33}$$

whose first three moments are, analogously to the equations (3.25), (3.26) and (3.27),

$$\rho(\boldsymbol{x}) = \int d^D\boldsymbol{\xi} f(\boldsymbol{\xi}), \tag{3.34}$$

$$\boldsymbol{u}(\boldsymbol{x}) = \frac{1}{\rho(\boldsymbol{x})} \int d^D\boldsymbol{\xi}\ \boldsymbol{\xi} f(\boldsymbol{\xi}), \text{ and,} \tag{3.35}$$

$$\frac{D}{2}\theta(\boldsymbol{x}) = \frac{1}{\rho(\boldsymbol{x})} \int d^D\boldsymbol{\xi}\ \frac{1}{2}\left[\boldsymbol{\xi} - \boldsymbol{u}(\boldsymbol{x})\right]^2 f(\boldsymbol{\xi}) \tag{3.36}$$

and the relation between the dimensionless and dimensional Maxwell-Boltzmann distribution functions are, respectively, $f(\boldsymbol{\xi}) \leftrightarrow f(\boldsymbol{\chi}) c_r^D$.

The reference temperature and the macroscopic velocity are the parameters that set the Taylor expansion. This means that the macroscopic velocity is small as compared to c_r and the temperature deviates very little from T_r. Therefore $\boldsymbol{u}(\boldsymbol{x})$ and $\theta(\boldsymbol{x})-1$ are small quantities no matter the point in space, fact that justifies a series expansion in powers of these quantities. Next we have to define a *single* small parameter ϵ to carry on the Taylor expansion as we shall take the expansion until order ϵ^2. The square of the macroscopic velocity and the temperature deviation will be considered of the same order: $|\boldsymbol{u}(\boldsymbol{x})| \sim \sqrt{\epsilon}$ and $\theta(\boldsymbol{x})-1 \sim \epsilon$. At this stage such choices seem rather arbitrary, but in the next chapter the Hermite polynomial expansion will bring understanding to them.

We have obtained a Taylor expansion of the Maxwell Boltzmann equilibrium distribution function (Eq.(3.33)) in powers of $T(\boldsymbol{x})/T_r - 1$ and $\boldsymbol{v(x)}/c_r$ up to the desired order of ϵ^2:

$$\begin{aligned}
\bar{f} \;=\; & \rho\omega(\boldsymbol{\xi})\Big\{1 + \boldsymbol{\xi}\cdot\boldsymbol{u} + \frac{1}{2}(\boldsymbol{\xi}\cdot\boldsymbol{u})^2 - \frac{\boldsymbol{u}^2}{2} + \frac{1}{2}(\theta-1)(\boldsymbol{\xi}^2 - D) + \frac{1}{6}(\boldsymbol{\xi}\cdot\boldsymbol{u})^3 \\
& -\frac{1}{2}\boldsymbol{u}^2(\boldsymbol{\xi}\cdot\boldsymbol{u}) + \frac{1}{2}(\theta-1)(\boldsymbol{\xi}\cdot\boldsymbol{u})(\boldsymbol{\xi}^2 - D - 2) + \frac{1}{24}(\boldsymbol{\xi}\cdot\boldsymbol{u})^4 + \frac{1}{8}\boldsymbol{u}^4 \\
& -\frac{1}{4}(\boldsymbol{\xi}\cdot\boldsymbol{u})^2\boldsymbol{u}^2 + \frac{1}{4}(\theta-1)\Big[(\boldsymbol{\xi}\cdot\boldsymbol{u})^2(\boldsymbol{\xi}^2 - D - 4) + \boldsymbol{u}^2(D + 2 - \boldsymbol{\xi}^2)\Big] \\
& +\frac{1}{8}(\theta-1)^2\Big[\boldsymbol{\xi}^4 - 2(D+2)\boldsymbol{\xi}^2 + D(D+2)\Big] + O(\epsilon^{5/2})\Big\},
\end{aligned} \tag{3.37}$$

where we have used the gaussian function

$$\omega(\boldsymbol{\xi}) \equiv \frac{1}{(2\pi)^{\frac{D}{2}}} \exp\left(-\frac{\boldsymbol{\xi}^2}{2}\right). \tag{3.38}$$

Remarkably, the three local parameters ρ, θ, and $\boldsymbol{u}$, contained in $\bar{f}$, are also its first three moments.

$$\rho(\boldsymbol{x}) = \int d^D\boldsymbol{\xi}\, \bar{f}(\boldsymbol{\xi}, \rho, \theta, \boldsymbol{u}), \tag{3.39}$$

$$\boldsymbol{u}(\boldsymbol{x}) = \frac{1}{\rho(\boldsymbol{x})} \int d^D\boldsymbol{\xi}\; \boldsymbol{\xi}\, \bar{f}(\boldsymbol{\xi}, \rho, \theta, \boldsymbol{u}), \text{ and,} \tag{3.40}$$

$$\frac{D}{2}\theta(\boldsymbol{x}) = \frac{1}{\rho(\boldsymbol{x})} \int d^D\boldsymbol{\xi}\; \frac{[\boldsymbol{\xi} - \boldsymbol{u}(\boldsymbol{x})]^2}{2} \bar{f}(\boldsymbol{\xi}, \rho, \theta, \boldsymbol{u}). \tag{3.41}$$

The parameters ρ, θ, and $\boldsymbol{u}$ are also the moments of the taylor expanded distribution function, thus keeping a property of the full Maxwell-Boltzmann distribution function. We shall see in the next chapter that this property stems from a mathematical structure anchored in the Hermite polynomials. Nevertheless to understand this property here it suffices to consider Eq.(A.16), given in appendix (A).

Next we taylor expand the full Maxwell-Boltzmann distribution function to obtain Eq.(3.37). A few remarks are worth of notice. The only scalars available are $\boldsymbol{\xi}\cdot\boldsymbol{u}$ and $\boldsymbol{u}^2$. The microscopic velocity $\boldsymbol{\xi}$ has no ϵ order assigned to it. In practice it can only take small values because of the gaussian decay. Therefore according to the set expansion criterion the only terms to be kept are those proportional to 1, $\boldsymbol{\xi}\cdot\boldsymbol{u}$, $\boldsymbol{u}^2$, $(\boldsymbol{\xi}\cdot\boldsymbol{u})^2$, $\boldsymbol{u}^3$, $(\boldsymbol{\xi}\cdot\boldsymbol{u})^2\boldsymbol{u}$, $(\boldsymbol{\xi}\cdot\boldsymbol{u})\boldsymbol{u}^2$, $(\boldsymbol{\xi}\cdot\boldsymbol{u})^3$, $\boldsymbol{u}^4$, $(\boldsymbol{\xi}\cdot\boldsymbol{u})^2\boldsymbol{u}^2$, $(\boldsymbol{\xi}\cdot\boldsymbol{u})^4$, $(\theta-1)$, $(\theta-1)\boldsymbol{\xi}\cdot\boldsymbol{u}$, $(\theta-1)\boldsymbol{u}^2$, $(\theta-1)(\boldsymbol{\xi}\cdot\boldsymbol{u})^2$, and $(\theta-1)^2$. Firstly consider small deviations of T_r, namely, $\theta = 1+(\theta-1)$ up to order ϵ^2 in the denominator of Eq.(3.33):

$$\frac{1}{\theta^{\frac{D}{2}}} = \frac{1}{[1+(\theta-1)]^{\frac{D}{2}}} = 1 - \frac{D}{2}(\theta-1) + \frac{D}{4}\frac{D+2}{2}(\theta-1)^2 + O(\epsilon^3). \tag{3.42}$$

The exponential also has a θ dependent denominator that must be expanded resulting in three different terms, which must be treated separately according to ϵ.

$$\begin{aligned} & \exp\left(-\frac{(\boldsymbol{\xi}-\boldsymbol{u})^2}{2\theta}\right) \\ = \;& \exp\left\{-\frac{(\boldsymbol{\xi}-\boldsymbol{u})^2}{2}\left[1-(\theta-1)+(\theta-1)^2+O(\epsilon^3)\right]\right\} \\ = \;& \exp\left[-\left(\frac{\boldsymbol{\xi}^2}{2}-\boldsymbol{\xi}\cdot\boldsymbol{u}+\frac{\boldsymbol{u}^2}{2}\right)\right]\cdot\exp\left[\left(\frac{\boldsymbol{\xi}^2}{2}-\boldsymbol{\xi}\cdot\boldsymbol{u}\frac{\boldsymbol{u}^2}{2}\right)(\theta-1)\right]\cdot \\ & \cdot\exp\left[-\left(\frac{\boldsymbol{\xi}^2}{2}-\boldsymbol{\xi}\cdot\boldsymbol{u}+\frac{\boldsymbol{u}^2}{2}\right)(\theta-1)^2\right]\ldots \end{aligned} \tag{3.43}$$

In the first exponential we factorize the gaussian function $\exp\left(-\boldsymbol{\xi}^2/2\right)$, because of its zeroth ϵ order. Next we select for the three exponentials only those terms of order equal

or lower than ϵ^2. The first exponential becomes

$$\exp\left[-\left(\frac{\boldsymbol{\xi}^2}{2}-\boldsymbol{\xi}\cdot\boldsymbol{u}+\frac{\boldsymbol{u}^2}{2}\right)\right]=\exp\left(-\frac{\boldsymbol{\xi}^2}{2}\right)\cdot[1+\boldsymbol{\xi}\cdot\boldsymbol{u}-\frac{\boldsymbol{u}^2}{2}+\frac{1}{2}(\boldsymbol{\xi}\cdot\boldsymbol{u})^2$$
$$-\frac{1}{2}(\boldsymbol{\xi}\cdot\boldsymbol{u})\boldsymbol{u}^2+\frac{\boldsymbol{u}^4}{8}+\frac{1}{6}(\boldsymbol{\xi}\cdot\boldsymbol{u})^3-\frac{1}{4}(\boldsymbol{\xi}\cdot\boldsymbol{u})^2\boldsymbol{u}^2+\frac{1}{24}(\boldsymbol{\xi}\cdot\boldsymbol{u})^4+O(\epsilon^{5/2})]. \quad (3.44)$$

The second one,

$$\exp\left[-\left(\frac{\boldsymbol{\xi}^2}{2}-\boldsymbol{\xi}\cdot\boldsymbol{u}+\frac{\boldsymbol{u}^2}{2}\right)(\theta-1)\right] \quad (3.45)$$
$$=\ 1+\left(\frac{\boldsymbol{\xi}^2}{2}-\boldsymbol{\xi}\cdot\boldsymbol{u}+\frac{\boldsymbol{u}^2}{2}\right)(\theta-1)+\frac{\boldsymbol{\xi}^4}{8}(\theta-1)^2+O(\epsilon^{5/2}),$$

and the third,

$$\exp\left[-\left(\frac{\boldsymbol{\xi}^2}{2}-\boldsymbol{\xi}\cdot\boldsymbol{u}+\frac{\boldsymbol{u}^2}{2}\right)(\theta-1)^2\right]=1-\frac{\boldsymbol{\xi}^2}{2}(\theta-1)^2+O(\epsilon^{5/2}). \quad (3.46)$$

The product of Eqs.(3.42) and (3.43), together with the expansions of Eq.(3.44), (3.45), (3.46), gives that

$$\begin{aligned} f \ =\ & \rho\omega(\boldsymbol{\xi})\left[1-\frac{D}{2}(\theta-1)+\frac{D}{4}\frac{D+2}{2}(\theta-1)^2-O(\epsilon^3)\right]\cdot\left[1+\boldsymbol{\xi}\cdot\boldsymbol{u}-\frac{\boldsymbol{u}^2}{2}\right. \\ & +\frac{1}{2}(\boldsymbol{\xi}\cdot\boldsymbol{u})^2-\frac{1}{2}(\boldsymbol{\xi}\cdot\boldsymbol{u})\boldsymbol{u}^2+\frac{\boldsymbol{u}^4}{8}+\frac{1}{6}(\boldsymbol{\xi}\cdot\vec{\boldsymbol{u}})^3-\frac{1}{4}(\boldsymbol{\xi}\cdot\boldsymbol{u})^2\boldsymbol{u}^2+\frac{1}{24}(\boldsymbol{\xi}\cdot\boldsymbol{u})^4 \\ & \left.-O(\epsilon^{5/2})\right]\cdot\left[1+\left(\frac{\boldsymbol{\xi}^2}{2}-\boldsymbol{\xi}\cdot\boldsymbol{u}+\frac{\boldsymbol{u}^2}{2}\right)(\theta-1)+\frac{\boldsymbol{\xi}^4}{8}(\theta-1)^2+O(\epsilon^{5/2})\right]\cdot \\ & \cdot\left[1-\frac{\boldsymbol{\xi}^2}{2}(\theta-1)^2+O(\epsilon^{5/2})\right]. \end{aligned} \quad (3.47)$$

Finally we expand Eq.(3.47) and hold terms up to order ϵ^2, by multiplying the ϵ expansions of the three exponentials of the numerator with that of the denominator to obtain Eq.(3.37).

3.3 The discretization of the microscopic velocity

A very old problem in Mathematics is to calculate the integral of a function, $\int g(x)dx$, in case it is not possible to perform the integration directly. Hence a general scheme

must be devised to obtain the integral of a general function $g(x)$ through other ways. Many formulas were developed for this purpose in the past, such as those of the kind, $\int g(x)dx = \sum_{i=1}^{N} g(x_i)w_i$ [1]. The integral is obtained just by sum of the function at N points x_i, times fixed weights w_i which are independent of the function $g(x)$ under consideration. This method was developed to approximately calculate areas and volumes. The method became known as the method of gaussian quadrature [3][2].

Gaussian quadrature is of fundamental relevance for a discrete treatment of the Boltzmann equation. The continuous microscopic velocity space of section 3.1.3 is made discrete by this approach. We are interested in integrating the gaussian function of Eq.(3.38) times a polynomial function. Then by the above method a integral in continuous velocity space is transformed *exactly* into a sum over discrete microscopic velocities [24], χ_α,

$$\int \omega(\boldsymbol{\chi}) h(\boldsymbol{\chi}) d^D\chi = \sum_\alpha w_\alpha h(\boldsymbol{\chi_\alpha}) \tag{3.48}$$

where $h(\boldsymbol{\chi})$ is a polynomial of $\boldsymbol{\chi_\alpha}$ takes over a discrete set of values, and $\omega(\boldsymbol{\chi})$ is a Gaussian weight function (see Eq.(3.38)). It remains to know the appropriate weights w_α. Thus, the equations (3.25), (3.26) and (3.27) become

$$\rho = \sum_\alpha f_\alpha = \sum_\alpha f_\alpha^{(0)}, \tag{3.49}$$

$$\rho \boldsymbol{v} = \sum_\alpha \boldsymbol{\chi_\alpha} f_\alpha = \sum_\alpha \boldsymbol{\chi_\alpha} f_\alpha^{(0)}, \text{ and} \tag{3.50}$$

$$\rho\varepsilon = \frac{1}{2}\sum_\alpha (\boldsymbol{\chi_\alpha} - \boldsymbol{v})^2 f_\alpha = \frac{1}{2}\sum_\alpha (\boldsymbol{\chi_\alpha} - \boldsymbol{v})^2 f_\alpha^{(0)}. \tag{3.51}$$

Notice that f_α has the unit of $f d^D\chi$.

The microscopic velocities are reduced to a set of discrete moduli and directions (see figure 3.2). This velocity set lives in the discretized position space which consists on a regular array of square (two-dimensions) and cubic (three-dimensions) cells. Given any point in position space, associated to it is the velocity set, which interconnects this point

[2]http://en.wikipedia.org/wiki/Gaussian_quadrature

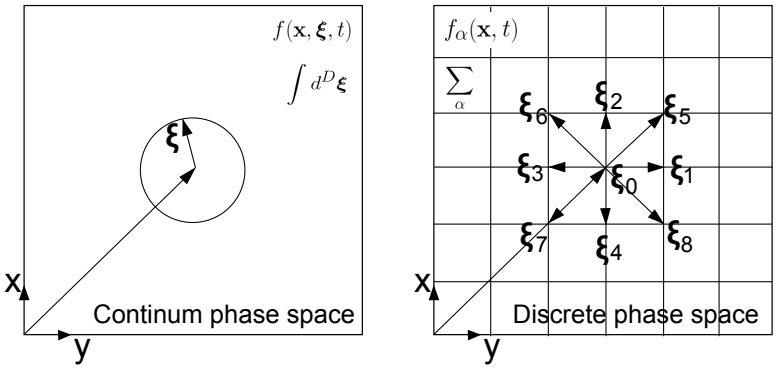

Figure 3.2: Ilustration of the continuum an discrete phase space. The discrete phase space is represented here by the D2V9 lattice.

to a selected set of nearest neighbor points. Therefore there is the position space regular, a lattice with an infinite number of points. There is also the discrete velocity lattice, formed by the a finite set of vectors, whose properties are best described through a example, as discussed below. These lattice vectors have to obey the following rules listed below [38]:

$$\sum_\alpha w_\alpha = 1 \tag{3.52}$$

$$\sum_\alpha w_\alpha \xi_\alpha^i = 0 \tag{3.53}$$

$$\sum_\alpha w_\alpha \xi_\alpha^i \xi_\alpha^j = \delta^{ij} \tag{3.54}$$

$$\sum_\alpha w_\alpha \xi_\alpha^i \xi_\alpha^j \xi_\alpha^k = 0 \tag{3.55}$$

$$\sum_\alpha w_\alpha \xi_\alpha^i \xi_\alpha^j \xi_\alpha^k \xi_\alpha^l = \delta^{ijkl} \tag{3.56}$$

$$\sum_\alpha w_\alpha \xi_\alpha^i \xi_\alpha^j \xi_\alpha^k \xi_\alpha^l \xi_\alpha^m = 0 \tag{3.57}$$

$$\sum_\alpha w_\alpha \xi_\alpha^i \xi_\alpha^j \xi_\alpha^k \xi_\alpha^l \xi_\alpha^m \xi_\alpha^n = \delta^{ijklmn}, \tag{3.58}$$

$$\vdots$$

$$\sum_\alpha w_\alpha \xi_\alpha^{i_1} \xi_\alpha^{i_2} \xi_\alpha^{i_3} \dots \xi_\alpha^{i_M} = \begin{cases} \delta^{i_1 i_2 i_3 \dots i_M} & \text{if M is even} \\ 0 & \text{if M is odd} \end{cases} \tag{3.59}$$

The $\delta^{\cdots}$ tensors are constructed recursively from the Kronecker's symbol: $\delta^{ij} = 1$ for $i = j$ and 0 for $i \neq j$. In case of four indices,

$$\delta^{ijkl} \equiv \delta^{ij}\delta^{kl} + \delta^{ik}\delta^{jl} + \delta^{il}\delta^{kj}. \tag{3.60}$$

The sixth order tensor is,

$$\delta^{ijklmn} \equiv \delta^{ij}\delta^{klmn} + \delta^{ik}\delta^{jlmn} + \delta^{il}\delta^{kjmn} + \delta^{im}\delta^{jkln} + \delta^{in}\delta^{jklm}. \tag{3.61}$$

The eight order is,

$$\begin{aligned}\delta^{ijklmnpq} \equiv \delta^{ij}\delta^{klmnpq} + \delta^{ik}\delta^{jlmnpq} + \delta^{il}\delta^{jkmnpq} + \\ +\delta^{im}\delta^{jklnpq} + \delta^{in}\delta^{jklmpq} + \delta^{ip}\delta^{jklmnq} + \delta^{iq}\delta^{jklmnp},\end{aligned} \tag{3.62}$$

and so forth.

The next goal is to determine the set of weights, w_α, and microscopic velocity components, ξ^i_α, that satisfy the above relations. Then an important aspect is the number of relations that must be satisfied, in other words, the value of M that must be taken. There is a criterion for this, based on the demand that the taylor expanded Maxwell-Boltzmann distribution upholds the property that its three free parameters are also the first three moments. For instance the construction of the non-thermal LBM done in the eighties only required $M = 5$, but for the thermal case this number must be higher, namely, $M = 9$. In appendix C, we see some examples of lattices and their respective number M. The lattices are named with the special notation DdVq, where d is the dimensions of space we are treating and q is the number of lattice vectors. These lattice vectors have to obey some rules so as it has a sufficiently isotropic behavior.

3.3.1 The D2V9 lattice

To illustrate the previously discussed rules for the construction of a discrete set of velocities, we study the example of the D2V9 lattice, which requires the use of the relations

of Eqs.(3.52)-(3.57) up to $M = 5$. Therefore this lattice can be used for the construction of a non-thermal LBM, but not for the thermal one.

Figure 3.3 shows a scheme of the D2V9 lattice and its discrete set of microscopical velocities $\boldsymbol{\xi_\alpha}$. Here we introduce another demand, we would like to have one particular vector, say that along the x-axis, to have unit length, $(1, 0)$. However we do not know if such condition is in conflict with equations (3.52)-(3.57). These equations surely allow for the choice of $(c_r, 0)$, where c_r is an arbitrary constant. This is equivalent to the definition of the new set $\boldsymbol{\chi_\alpha} = \boldsymbol{\xi_\alpha} c_r$ that obeys equations (3.52)-(3.57) provided that the following substitution is taken, $\boldsymbol{\xi_\alpha} \rightarrow \boldsymbol{\chi_\alpha}$ and $\delta^{i_1 i_2 i_3 \ldots i_M} \rightarrow c_r^M \, \delta^{i_1 i_2 i_3 \ldots i_M}$. Concerning the D2V9 lattice we find that the following set is possible: $\boldsymbol{\chi_0} = (0, 0)$, $\boldsymbol{\chi_1} = (1, 0)$, $\boldsymbol{\chi_2} = (0, 1)$, $\boldsymbol{\chi_3} = (-1, 0)$, $\boldsymbol{\chi_4} = (0, -1)$, $\boldsymbol{\chi_5} = (1, 1)$, $\boldsymbol{\chi_6} = (-1, 1)$, $\boldsymbol{\chi_7} = (-1, -1)$, $\boldsymbol{\chi_8} = (1, -1)$. Now we will use equations (3.52), (3.54), and (3.56) to find the weights w_α and the constant c_r for the D2V9 lattice.

It follows that weights of velocity vectors with the same moduli are equal.

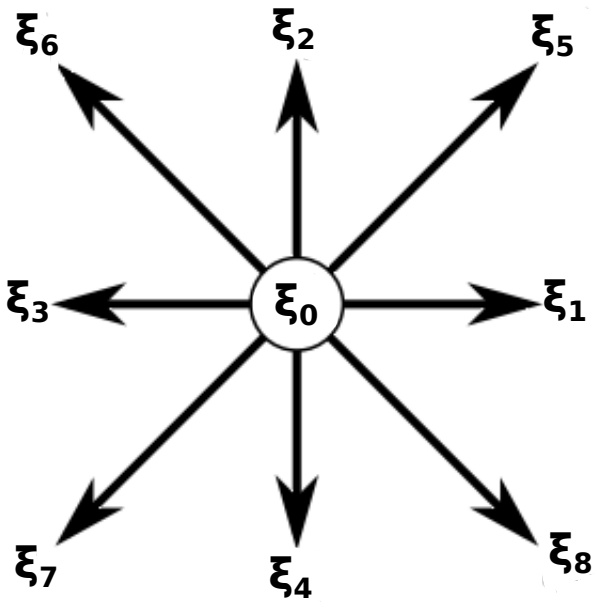

Figure 3.3: The D2V9 lattice with indication of discrete velocity.

$$w_\alpha = \begin{cases} w_0 & \text{for} \quad \alpha = 0 \\ w_s & \text{for} \quad \alpha = 1,2,3,4 \\ w_l & \text{for} \quad \alpha = 5,6,7,8 \end{cases} \tag{3.63}$$

Using Eq.(3.52),

$$\sum_{\alpha=0}^{8} w_\alpha = 1 \Rightarrow w_0 + 4w_s + 4w_l = 1. \tag{3.64}$$

From Eq.(3.54)

$$\sum_{\alpha=0}^{8} w_\alpha \chi_\alpha^i \chi_\alpha^j = c_r^2 \delta^{ij}.$$

In two dimensions, we can have $i = x$ or y and $j = x$ or y, but if $x \neq y$ we obtain a trivial result. We also have that, due to space isotropy, the directions x and y are equivalent. So we calculate the above sum for $i = j = x$

$$\begin{aligned} &w_0(\chi_0^x)^2 + w_1(\chi_1^x)^2 + w_2(\chi_2^x)^2 + w_3(\chi_3^x)^2 + w_4(\chi_4^x)^2 \\ &+w_5(\chi_5^x)^2 + w_6(\chi_6^x)^2 + w_7(\chi_7^x)^2 + w_8(\chi_8^x)^2 = c_r^2 \\ &\Rightarrow 2w_s + 4w_l = c_r^2. \end{aligned} \tag{3.65}$$

And from Eq.(3.56)

$$\sum_{\alpha=0}^{8} w_\alpha \chi_\alpha^i \chi_\alpha^j \chi_\alpha^k \chi_\alpha^l = c_r^4 (\delta^{ij}\delta^{kl} + \delta^{ik}\delta^{jl} + \delta^{il}\delta^{jk}). \tag{3.66}$$

The only two cases that give relevant equations is when all the directions are the same $i = j = k = l$ or when they are equal in pairs, for example $i = j \neq k = l$. For the first case, with all components in x direction

$$\begin{aligned} &w_0(\chi_0^x)^4 + w_1(\chi_1^x)^4 + w_2(\chi_2^x)^4 + w_3(\chi_3^x)^4 + w_4(\chi_4^x)^4 \\ &+w_5(\chi_5^x)^4 + w_6(\chi_6^x)^4 + w_7(\chi_7^x)^4 + w_8(\chi_8^x)^4 = 3c_r^4 \\ &\Rightarrow 2w_s + 4w_l = 3c_r^4, \end{aligned} \tag{3.67}$$

and for the second case, with $(i = j = x) \neq (k = l = y)$

$$\begin{aligned} &w_0(\chi_0^x)^2(\chi_0^y)^2 + w_1(\chi_1^x)^2(\chi_1^y)^2 + w_2(\chi_2^x)^2(\chi_2^y)^2 + w_3(\chi_3^x)^2(\chi_3^y)^2 + w_4(\chi_4^x)^2(\chi_4^y)^2 \\ &+w_5(\chi_5^x)^2(\chi_5^y)^2 + w_6(\chi_6^x)^2(\chi_6^y)^2 + w_7(\chi_7^x)^2(\chi_7^y)^2 + w_8(\chi_8^x)^2(\chi_8^y)^2 = c_r^4 \end{aligned}$$

$$\Rightarrow 4w_l = c_r^4 \tag{3.68}$$

Therefore we have a system of four equations:

$$\begin{cases} w_0 + 4w_s + 4w_l = 1 \\ 2w_s + 4w_l = c_r^2 \\ 2w_s + 4w_l = 3c_r^4 \\ 4w_l = c_r^4 \end{cases} \tag{3.69}$$

which has the solution

$$w_0 = \frac{4}{9},\ w_s = \frac{1}{9},\ w_l = \frac{1}{36},\ c_r = \frac{1}{\sqrt{3}} \tag{3.70}$$

Therefore we have determined all the weights, w_α, and the reference velocity, c_r, of the D2V9 lattice, that are summarized in table C.2. This reference velocity c_r is just a number contrary to that one defined in Eq.(3.30), which is a dimensional physical velocity. Yet they both have the same application since they define the speed of sound both in dimensional and dimensionless units. c_r acquires a different value for each lattice.

Once in power of the weights, one can proceed to calculate the macroscopic quantities in equations (3.49), (3.50) and (3.51) with the distribution function calculated in section 3.2 but now with a well defined set of velocities vectors $\boldsymbol{\chi_\alpha}$.

$$\begin{aligned} f_\alpha^{(0)} \;=\; & \rho w_\alpha \Bigg\{ 1 + \frac{\boldsymbol{\chi_\alpha}\cdot\boldsymbol{u}}{c_r} + \frac{1}{2}\frac{(\boldsymbol{\chi_\alpha}\cdot\boldsymbol{u})^2}{c_r^2} - \frac{\boldsymbol{u}^2}{2} + \frac{1}{2}(\theta-1)\Big(\frac{\boldsymbol{\chi_\alpha}^2}{c_r^2} - D\Big) + \frac{1}{6}\frac{(\boldsymbol{\chi_\alpha}\cdot\boldsymbol{u})^3}{c_r^3} \\ & -\frac{1}{2}\boldsymbol{u}^2\frac{(\boldsymbol{\chi_\alpha}\cdot\boldsymbol{u})}{c_r} + \frac{1}{2}(\theta-1)\frac{(\boldsymbol{\chi_\alpha}\cdot\boldsymbol{u})}{c_r}\Big(\frac{\boldsymbol{\chi_\alpha}^2}{c_r^2} - D - 2\Big) - \frac{1}{4}\frac{(\boldsymbol{\chi_\alpha}\cdot\boldsymbol{u})^2}{c_r^2}\boldsymbol{u}^2 + \frac{1}{8}\boldsymbol{u}^4 \\ & +\frac{1}{24}\frac{(\boldsymbol{\chi_\alpha}\cdot\boldsymbol{u})^4}{c_r^4} + \frac{1}{4}(\theta-1)\Big[\frac{(\boldsymbol{\chi_\alpha}\cdot\boldsymbol{u})^2}{c_r^2}\Big(\frac{\boldsymbol{\chi_\alpha}^2}{c_r^2} - D - 4\Big) + \boldsymbol{u}^2\Big(D + 2 - \frac{\boldsymbol{\chi_\alpha}^2}{c_r^2}\Big)\Big] \\ & +\frac{1}{8}(\theta-1)^2\Big[\frac{\boldsymbol{\chi_\alpha}^4}{c_r^4} - 2(D+2)\frac{\boldsymbol{\chi_\alpha}^2}{c_r^2} + D(D+2)\Big]\Bigg\} \end{aligned} \tag{3.71}$$

To construct a LBM computational code able to treat the thermal compressible fluid through a BGK-Boltzmann equation, one must use lattices that satisfy at least the $M = 7$ level conditions. This is the case of the D2V17 lattice. The D2V37 lattice, treated by Siebert et. al [33], satisfies the $M = 9$ relations and also can be used to study the thermal

compressible flow. In appendix C we see in more details the properties of such lattices as well as other one, two and three dimensional lattices. The corresponding sets of discrete velocities, weights and reduced velocity are given there.

3.4 The lattice Boltzmann method

In this section we provide a description of the numerical algorithm associated to the lattice Boltzmann method for computational purposes. Position space is made of a regular lattice such that to each of its points there is an associated local distribution function $f_\alpha(\mathbf{x}, t)$. Knowledge of these functions determines the macroscopic quantities in position space.

We conveniently write the discrete Boltzmann equation (3.24) in two steps,

$$f_\alpha^{aux}(\boldsymbol{x}, t + \Delta t) = f_\alpha(\boldsymbol{x}, t) - \frac{1}{\tau}[f_\alpha(\boldsymbol{x}, t) - f_\alpha^{(0)}(\boldsymbol{x}, t)], \tag{3.72}$$

$$f_\alpha(\boldsymbol{x} + \boldsymbol{\xi_\alpha}\Delta t, t + \Delta t) = f_\alpha^{aux}(\boldsymbol{x}, t + \Delta t) \tag{3.73}$$

by introducing a *auxiliary* distribution function $f_\alpha^{aux}(\boldsymbol{x}, t)$. These two steps can be interpreted as collision and streaming of fictitious particles, respectively.

The basic algorithm can be summarized as follows[3] [19, 36]:

a) Initial conditions: The macroscopic variables ρ, $\boldsymbol{u}$ and θ are initialized to given values in $f_\alpha^{(0)}(\boldsymbol{x}, t)$.

b) Collision: The Eq.(3.72) describes how the distribution function changes at each node, as if it had undergone a collision.

c) Streaming: The Eq.(3.73) gives the evolution of the distribution function for a time step Δt, as if it had undergone a propagation.

So, in the streaming step we move the direction-specific function f_α to the nearest neighbor lattice nodes, as shown in figure 3.4.

[3] See *http://en.wikipedia.org/wiki/Lattice_Boltzmann_methods* and *http://www.cims.nyu.edu/∼billbao/report930.pdf*

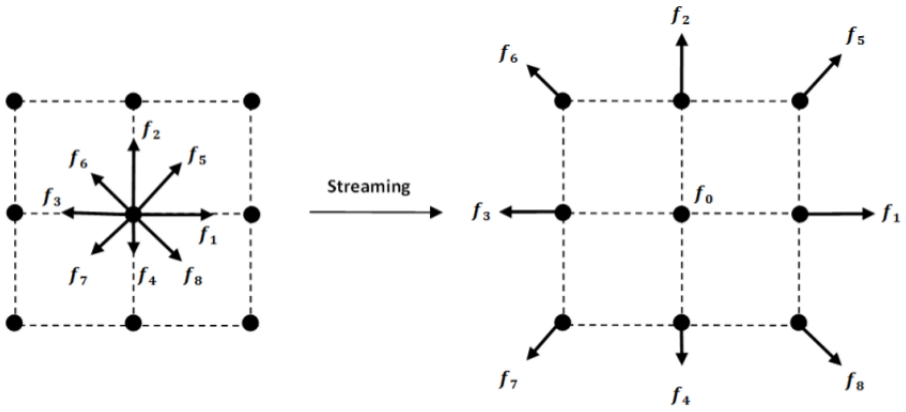

Figure 3.4: Illustration for streaming step for D2V9 lattice.

d) Macroscopic quantities: Using equations (3.39), (3.40) and (3.41) and the weights of the lattice we can calculate the moments

$$\rho = \sum_{\alpha} f_{\alpha}, \tag{3.74}$$

$$\boldsymbol{u} = \frac{1}{\rho} \sum_{\alpha} \boldsymbol{\xi_{\alpha}} f_{\alpha}, \text{ and} \tag{3.75}$$

$$\frac{D}{2}\theta = \frac{1}{\rho} \sum_{\alpha} (\boldsymbol{\xi_{\alpha}} - \boldsymbol{u})^2 f_{\alpha}. \tag{3.76}$$

e) Equilibrium function: Once in power of these three moments, we go introduce them in the equilibrium distribution function of Eq.(3.71), thanks to the fact that the Chapman-Enskog relations hold.

f) Repeat from **b** to **e** for each step time until you want.

The steps from **b** to **e** can be cyclically permuted.

3.5 Macroscopic equations

The lattice Boltzmann method, using the distribution function in Eq.(3.71) together with the relations (3.52)-(3.59) provides a consistent scheme to describe the thermal compressible fluid. Its time evolution updates the local temperature, θ, density ρ, and macroscopic velocity $\boldsymbol{u}$. The question addressed here is what are macroscopic hydrodynamical

equations satisfied by these variables. A few years ago Siebert and collaborators [34] showed that they are exactly those of Landau & Lifshtz's book, obtained by general principles of mechanics and thermodynamics and previously described in chapter 2.

We will obtain in the next chapter the macroscopic hydrodynamical equations from the Boltzmann equations for the case of the quantum fluid, whose classical limit corresponds to the present situation.

Chapter 4

The quantum fluid

In this chapter we derive the major result of this thesis, which is a consistent LBM for quantum fluids. The LBM was formulated in the eighties originally to describe non-thermal classical fluids, and shown to be a second order Hermite expansion of the distribution function. It took nearly twenty five years to show here that quantum fluids can be treated similarly, namely, by a fourth order expansion instead. Siebert et al. has shown in 2007 that the classical thermal fluid also requires the fourth order expansion [34].

Therefore our first goal is to perform the Hermite polynomial expansion of the BE and FD equilibrium distribution functions to fourth order. Next we obtain the macroscopic hydrodynamical equations for the quantum fluid in terms of the temperature θ, the velocity u^i, and the chemical potential μ [32], as a result of the Chapman-Enskog analysis done in the BGK-Boltzmann equation. Instead of the chemical potential, the fugacity can be used, being defined as,

$$z \equiv e^{\frac{\mu}{\theta}}. \tag{4.1}$$

We notice that the hydrodynamical equations were derived for the BE-FD statistics long ago by E. A. Uheling and G. E. Uhlenbeck [37]. They started from the Boltzmann equation with a binary collision operator while here the starting point is the BGK collision operator, which, as a matter of fact, was only proposed decades after (fifties) the E. A. Uheling and G. E. Uhlenbeck study (thirties). we are not aware of any attempt to solve

the macroscopic hydrodynamical equations of E. A. Uheling and G. E. Uhlenbeck. These authors hoped that their viscosity and heat conductivity coefficients, obtained from the Boltzmann equation with quantum statistics, would provide a "test of the existence of Einstein-Bose statistics in real gases, as is required by theory". It seems to be also true that such macroscopic hydrodynamical equations were never applied to the treatment of electrons in metals, which are known to satisfy the BGK-Boltzmann equation with quantum statistics, according to Sommerfeld's theory [20]. The electrons inside a metal behave nearly as $T = 0$ fermions, as the ratio between room temperature (nearly three hundred Kelvin) and the Fermi surface temperature (nearly ten thousand Kelvin) is very small. Thus after eighty years of the E. A. Uheling and G. E. Uhlenbeck, we propose here a numerical method to describe Bose-Einstein condensate (BEC) and electrons in metals as fluids, similarly to liquids.

A remarkable feature of the macroscopic hydrodynamical equations of the quantum fluids is their similarity to the classical ones, provided that some auxiliary variables are introduced, starting with the pseudo-temperature defined below

$$\bar{\theta} = \theta \frac{g_{\frac{D}{2}+1}(z)}{g_{\frac{D}{2}}(z)}, \tag{4.2}$$

where,

$$g_\nu(z) \equiv \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1}\, dx}{z^{-1}e^x \pm 1}. \tag{4.3}$$

is the Fermi-Dirac integral (up sign, $+$) or the Bose-Einstein integral (down sign, $-$) [23]. This mapping of the quantum into the classical fluid is only spoiled by a term present in the pseudo heat flux vector, as shown below. Without the presence of this term the quantum fluid could be fully mapped into the classical fluid.

The quantum fluids becomes the classical one in the limit that BE and FD statistics become the MB statistics. In this limit $z^{-1}e^x \pm 1 \approx z^{-1}e^x$, thus the term ± 1 becomes

irrelevant in the denominator. Since

$$\Gamma(\nu) = \int_0^\infty e^{-x} x^{\nu-1}\, dx,$$

one obtains that $g_\nu(z) \approx z$ for the MB limit. Thus we conclude that in the classical limit the pseudo-temperature is the temperature itself. The BE-FD density is not an independent parameter, as in the MB case, but a function of the the temperature θ and the fugacity z,

$$\rho = (2\pi\theta)^{\frac{D}{2}} g_{\frac{D}{2}}(z). \tag{4.4}$$

Based on the above definitions of ρ and $\bar{\theta}$ we introduce the pseudo viscosity stress tensor for null volumetric viscosity, $\zeta = 0$,

$$\bar{\sigma}^{ij} \equiv \bar{\eta}\left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i} - \frac{2}{D}\delta^{ij}\frac{\partial u^l}{\partial x^l}\right), \tag{4.5}$$

which depends on the pseudo dynamic viscosity defined as,

$$\bar{\eta} \equiv \rho\bar{\theta}\tau\left(1 - \frac{\Delta t}{2\tau}\right). \tag{4.6}$$

We also define the pseudo thermal conductivity,

$$\bar{\kappa} \equiv \frac{D+2}{2}\rho\bar{\theta}\tau\left(1 - \frac{\Delta t}{2\tau}\right). \tag{4.7}$$

Their ratio is constant, $\bar{\kappa}/\bar{\eta} = (D+2)/2$, meaning that, like in the MB case, thermal and mechanical transfers are done by the same distribution and at the same rate, as there is only one BGK time relaxation parameter. We find others pseudo-variables during the chapter.

4.1 Expansion of the quantum equilibrium distribution functions by Hermite polynomials to N=4 order

In this section we derive the equilibrium distribution functions of quantum fluids by a Hermite polynomial expansion to $N = 4$ order. Consider the BE and FD distribution

functions, given by,

$$f^{(0)}(\boldsymbol{\chi}) = \frac{1}{\exp\left[\frac{(\boldsymbol{\chi}-\boldsymbol{v})^2 m}{2k_B T} - \frac{\mu'}{k_B T}\right] \pm 1}, \tag{4.8}$$

which depend on the microscopic velocity $\boldsymbol{\chi}$ and other three locally defined quantities, namely, the temperature $T(\boldsymbol{x})$, the macroscopic velocity $\boldsymbol{v}(\boldsymbol{x})$ and the chemical potential $\mu'(\boldsymbol{x})$.

Similarly to the last chapter here we also introduce dimensionless quantities, based on a reference temperature T_r, and a reference velocity:

$$c_r \equiv \sqrt{\frac{kT_r}{m}}, \tag{4.9}$$

both not present in the original BE-FD equilibrium distribution functions. Then the dimensionless temperature is

$$\theta \equiv \frac{T}{T_r}, \tag{4.10}$$

and the microscopic and macroscopic dimensionless velocities are defined as

$$\boldsymbol{\xi} \equiv \frac{\boldsymbol{\chi}}{c_r}, \text{ and } \boldsymbol{u} \equiv \frac{\boldsymbol{v}}{c_r}. \tag{4.11}$$

The dimensionless chemical potential is,

$$\mu \equiv \frac{\mu'}{k_B T_r}, \tag{4.12}$$

and the fugacity can be expressed in two ways,

$$z \equiv e^{\frac{\mu'}{k_B T}} = e^{\frac{\mu}{\theta}}. \tag{4.13}$$

The BE-FD function expressed in terms of dimensionless parameters becomes,

$$f^{(0)}(\boldsymbol{\xi}) = \frac{1}{z^{-1}\exp\left[\frac{(\boldsymbol{\xi}-\boldsymbol{u})^2}{2\theta}\right] \pm 1}. \tag{4.14}$$

The first three moments of the BE-FD function, obtained by integrating over the microscopic velocity $\boldsymbol{\chi}$, give that,

$$n(\boldsymbol{x}) = m\left(\frac{m}{2\pi\hbar}\right)^D \int d^D\boldsymbol{\chi}\, f^{(0)}(\boldsymbol{\chi}), \tag{4.15}$$

$$\boldsymbol{v}(\boldsymbol{x}) = \frac{1}{n(\boldsymbol{x})} \int d^D\boldsymbol{\chi}\ \boldsymbol{\chi} f^{(0)}(\boldsymbol{\chi}), \text{ and} \tag{4.16}$$

$$\frac{D}{2} k_B \bar{T}(\boldsymbol{x}) = \frac{1}{n(\boldsymbol{x})} \int d^D\boldsymbol{\chi}\ \frac{1}{2} m \left[\boldsymbol{\chi} - \boldsymbol{v}(\boldsymbol{x})\right]^2 f^{(0)}(\boldsymbol{\chi}). \tag{4.17}$$

We define the pseudo temperature $\bar{T}$ because the third moment is the internal energy, $\varepsilon = Dk_B\bar{T}/2$, and in the classical case we know that $\bar{T} = T$. Notice that the density n has the dimension of a D dimensional space density, as expected, namely, of $mass/(length)^D$, because $mv/2\pi\hbar$ has the dimension of $length^{-1}$. Thus through the following constant, which has the dimension of density,

$$n_0 \equiv m \left(\frac{mc_r}{2\pi\hbar}\right)^D. \tag{4.18}$$

By taking averages over the quantum equilibrium distribution function we obtain the dimensionless density ρ of Eq.(4.4), the macroscopic velocity $\boldsymbol{u}$, and the pseudo-temperature $\bar{\theta}$ of Eq.(4.2):

$$\rho(\boldsymbol{x}) \equiv \frac{n(\boldsymbol{x})}{n_0} = \int d^D\boldsymbol{\xi}\ f^{(0)}(\boldsymbol{\xi}), \tag{4.19}$$

$$\boldsymbol{u}(\boldsymbol{x}) = \frac{1}{\rho(\boldsymbol{x})} \int d^D\boldsymbol{\xi}\ \boldsymbol{\xi} f^{(0)}(\boldsymbol{\xi}), \text{ and} \tag{4.20}$$

$$\frac{D}{2} \bar{\theta}(\boldsymbol{x}) = \frac{1}{\rho(\boldsymbol{x})} \int d^D\boldsymbol{\xi}\ \frac{1}{2} \left[\boldsymbol{\xi} - \boldsymbol{u}(\boldsymbol{x})\right]^2 f^{(0)}(\boldsymbol{\xi}). \tag{4.21}$$

The explicit calculation of these moments are done below.

The decomposition of the BE-FD equilibrium distribution function $f^{(0)}$ of Eq.(4.14) means to write it in powers of Hermite polynomials (see appendix A):

$$f^{(0)}(\boldsymbol{x}, \boldsymbol{\xi}) = \omega(\boldsymbol{\xi}) \sum_{N=0}^{\infty} \frac{1}{N!} a^{i_1 i_2 \ldots i_N}(\boldsymbol{x}) H^{i_1 i_2 \ldots i_N}(\boldsymbol{\xi}). \tag{4.22}$$

Notice that this decomposition splits the dependence on the variables since the dimensionless microscopic velocity now falls entirely into the Hermite polynomials. The coefficients

of this expansion carry all the information about the local macroscopic fields. For this reason the following notation is employed, $a^{i_1\,i_2\ldots i_N}(\boldsymbol{x}) \equiv a^{i_1\,i_2\ldots i_N}[z(\boldsymbol{x}), \boldsymbol{u}(\boldsymbol{x}), \theta(\boldsymbol{x})]$. Applying the orthonormality of the Hermite polynomials, Eq.(A.3), one obtains an expression for the coefficients:

$$a^{i_1 i_2 \ldots i_N}(\boldsymbol{x}) = \int f^{(0)}(\boldsymbol{x}, \boldsymbol{\xi}) H^{i_1 i_2 \ldots i_N}(\boldsymbol{\xi}) d^D\boldsymbol{\xi}. \tag{4.23}$$

Notice that the BE-FD function is even in the difference between the macroscopic and the microscopic velocities, $f^{(0)}(\boldsymbol{x}, \boldsymbol{\xi} - \boldsymbol{u}) = f^{(0)}(\boldsymbol{x}, \boldsymbol{u} - \boldsymbol{\xi})$, a helpful property to compute the coefficients of Eq.(4.23). Then the coefficient associated to any odd Hermite polynomial vanishes since $\int d^D\boldsymbol{\xi}\, f(\boldsymbol{\xi} - \boldsymbol{u}) H^{i_1 \ldots i_{2L+1}}(\boldsymbol{\xi} - \boldsymbol{u}) = 0$. A discussion of such properties is done in the appendix A. We introduce the variable $\boldsymbol{\eta} = \boldsymbol{\xi} - \boldsymbol{u}$ and write the BE-FD distribution function as $f(\boldsymbol{\eta}) = 1/\left(z^{-1} e^{\frac{\eta^2}{2\theta}} \pm 1\right)$ to express the coefficients as,

$$a^{i_1 i_2 \ldots i_N} = \int f^{(0)}(\boldsymbol{\eta}) H^{i_1 i_2 \ldots i_N}(\boldsymbol{\xi}) d^D\boldsymbol{\eta}. \tag{4.24}$$

Coefficient N=0

To obtain the lowest Hermite coefficient we integrate in D dimensions

$$a = \int \frac{H d^D\eta}{z^{-1} e^{\frac{\eta^2}{2\theta}} \pm 1}. \tag{4.25}$$

In D dimensions, the D-spherical coordinates are of the form[1]

$$y_1 = r \cos\phi_1 \tag{4.26}$$

$$y_2 = r \sin\phi_1 \cos\phi_2 \tag{4.27}$$

$$y_3 = r \sin\phi_1 \sin\phi_2 \cos\phi_3 \tag{4.28}$$

$$\vdots$$

$$y_{D-1} = r \sin\phi_1 \ldots \sin\phi_{D-2} \cos\phi_{D-1} \tag{4.29}$$

$$y_D = r \sin\phi_1 \ldots \sin\phi_{D-2} \sin\phi_{D-1} \tag{4.30}$$

[1] See *http://en.wikipedia.org/wiki/N-sphere* for instance.

$$d^D y = r^{D-1}\sin^{D-2}\phi_1 \sin^{D-3}\phi_2 ... \sin\phi_{D-2}\, dr\, d\phi_1\, d\phi_2\, ...d\phi_{D-1} \tag{4.31}$$

So the coefficient becomes

$$a = \int \frac{H d^D\eta}{z^{-1}e^{\frac{\eta^2}{2\theta}} \pm 1} = C_1 \int_0^\infty \frac{\eta^{D-1} d\eta}{z^{-1}e^{\frac{\eta^2}{2\theta}} \pm 1}, \tag{4.32}$$

where C_1 is the angular integral, given by

$$C_1 \equiv \int_{\phi_{D-1}=0}^{2\pi}\int_{\phi_{D-2}=0}^{\pi} ... \int_{\phi_1=0}^{\pi} \sin^{D-2}\phi_1 \sin^{D-3}\phi_2 ... \sin\phi_{D-2}\, d\phi_1\, d\phi_2 ... d\phi_{D-1}. \tag{4.33}$$

But the volume of a n-sphere of radius r is

$$V_D(r) = \frac{\pi^{D/2}}{\Gamma\left(\frac{D}{2}+1\right)} r^D, \tag{4.34}$$

and the volume of the spherical shell (volume element) is

$$d^D r = \frac{D\pi^{\frac{D}{2}}}{\Gamma\left(\frac{D}{2}+1\right)} r^{D-1} dr. \tag{4.35}$$

Making the angular integration in Eq.(4.31) we obtain $C_1 r^{D-1} dr$, that is exactly the volume of spherical shell in Eq.(4.35). So C_1 is

$$C_1 = \frac{D\pi^{\frac{D}{2}}}{\Gamma\left(\frac{D}{2}+1\right)}, \tag{4.36}$$

making the substitution $x = \eta^2/2\theta$, the differential stay $d\eta = \frac{\sqrt{2\theta}}{2} x^{-1/2} dx$

$$a = C_1 \frac{(2\theta)^{\frac{D}{2}}}{2} \Gamma\left(\frac{D}{2}\right) g_{\frac{D}{2}}(z) = (2\pi)^{\frac{D}{2}} \theta^{\frac{D}{2}} g_{\frac{D}{2}}(z) \equiv \rho \tag{4.37}$$

since we have the property of gamma functions $\Gamma(t+1) = t\Gamma(t)$. This coefficient is the density itself, $a = \rho = \int d^D\boldsymbol{\xi}\, f^{(0)}(\boldsymbol{\xi})$, as given by Eq.(4.4).

Coefficient N=1

To obtain this coefficient take Eq.(A.20) such that,

$$\begin{aligned} a^i &= \int f^{(0)}(\boldsymbol{\eta}) H^i(\boldsymbol{\xi}) d^D\boldsymbol{\eta} \\ &= \int f^{(0)}(\boldsymbol{\eta}) \left[H^i(\boldsymbol{\eta}) + H u^i\right] d^D\boldsymbol{\eta} = u^i \int f^{(0)}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} \\ &= u^i \rho \end{aligned} \tag{4.38}$$

as the first integral vanishes because it is odd. Using analogous arguments, we find the next coefficients.

Coefficient N=2

One gets from Eq.(A.21) that,

$$\begin{aligned} a^{ij} &= \int f^{(0)}(\boldsymbol{\eta}) H^{ij}(\boldsymbol{\xi}) d^D\boldsymbol{\eta} \qquad (4.39)\\ &= \int f^{(0)}(\boldsymbol{\eta}) \left[H^{ij}(\boldsymbol{\eta}) + u^i H^j(\boldsymbol{\eta}) + u^j H^i(\boldsymbol{\eta}) + u^i u^j H\right] d^D\boldsymbol{\eta} \\ &= \int f^{(0)}(\boldsymbol{\eta}) H^{ij}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} + \rho u^i u^j. \qquad (4.40) \end{aligned}$$

The terms proportional to u^j vanish because of the odd integrals and it remains to calculate the integrals below.

$$\int f^{(0)}(\boldsymbol{\eta}) \eta^i \eta^j d^D\boldsymbol{\eta} = \frac{\delta^{ij}}{D} \int f^{(0)}(\boldsymbol{\eta}) \eta^2 d^D\boldsymbol{\eta} = \theta\rho \frac{g_{\frac{D}{2}+1}(z)}{g_{\frac{D}{2}}(z)} \delta^{ij}. \qquad (4.41)$$

The other integral to compute is,

$$\int f^{(0)}(\boldsymbol{\eta}) H^{ij}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} = \rho\delta^{ij} \left(\theta \frac{g_{\frac{D}{2}+1}(z)}{g_{\frac{D}{2}}(z)} - 1 \right). \qquad (4.42)$$

Introducing the pseudo temperature of Eq.(4.2), the second order coefficient becomes,

$$a^{ij} = \rho \left[\delta^{ij} \left(\bar{\theta} - 1\right) + u^i u^j\right]. \qquad (4.43)$$

Hereafter we directly use Eq.(4.2) to shorten the notation.

Coefficient N=3

One gets from Eq.(A.22) that,

$$\begin{aligned} a^{ijk} &= \int f^{(0)}(\boldsymbol{\eta}) H^{ijk}(\boldsymbol{\xi}) d^D\boldsymbol{\eta} \\ &= \int f^{(0)}(\boldsymbol{\eta}) \left[H^{ijk}(\boldsymbol{\eta}) + u^i H^{jk}(\boldsymbol{\eta}) + u^j H^{ik}(\boldsymbol{\eta}) + u^k H^{ij}(\boldsymbol{\eta}) \right. \\ &\quad \left. + u^i u^j H^k(\boldsymbol{\eta}) + u^i u^k H^j(\boldsymbol{\eta}) + u^j u^k H^i(\boldsymbol{\eta}) + u^i u^j u^k H\right] d^D\boldsymbol{\eta} \\ &= \rho \left[(u^i\delta^{jk} + u^j\delta^{ik} + u^k\delta^{ij})\bar{\theta} + u^i u^j u^k\right]. \end{aligned} \qquad (4.44)$$

Terms proportional to $u^i u^j$ vanish because they are proportional to integrals over a Hermite polynomial of odd order.

Coefficient N=4

One gets from Eq.(A.23) that,

$$\begin{aligned} a^{ijkl} &= \int f^{(0)}(\boldsymbol{\eta}) H^{ijkl}(\boldsymbol{\xi}) d^D\boldsymbol{\eta} \\ &= \int f^{(0)}(\boldsymbol{\eta}) \left[H^{ijkl}(\boldsymbol{\eta}) + u^i H^{jkl}(\boldsymbol{\eta}) + u^j H^{ijk}(\boldsymbol{\eta}) + u^k H^{ijl}(\boldsymbol{\eta}) \right. \\ &\quad + u^l H^{ijk}(\boldsymbol{\eta}) + u^i u^j H^{kl}(\boldsymbol{\eta}) + u^i u^k H^{jl}(\boldsymbol{\eta}) + u^i u^l H^{jk}(\boldsymbol{\eta}) + u^k u^l H^{ij}(\boldsymbol{\eta}) \\ &\quad + u^j u^l H^{ik}(\boldsymbol{\eta}) + u^j u^k H^{il}(\boldsymbol{\eta}) + u^i u^j u^k H^l(\boldsymbol{\eta}) + u^i u^j u^l H^k(\boldsymbol{\eta}) \\ &\quad \left. + u^j u^k u^l H^i(\boldsymbol{\eta}) + u^i u^k u^l H^j(\boldsymbol{\eta}) + u^i u^j u^k u^l H \right] d^D\boldsymbol{\eta}. \end{aligned} \tag{4.45}$$

Because of the odd integrals the terms proportional to u^j and $u^i u^j u^k$ do not contribute, and so,

$$\begin{aligned} a^{ijkl} &= \int f^{(0)}(\boldsymbol{\eta}) H^{ijkl}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} \\ &\quad + u^i u^j \int f^{(0)}(\boldsymbol{\eta}) H^{kl}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} + u^i u^k \int f^{(0)}(\boldsymbol{\eta}) H^{jl}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} \\ &\quad + u^i u^l \int f^{(0)}(\boldsymbol{\eta}) H^{jk}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} + u^k u^l \int f^{(0)}(\boldsymbol{\eta}) H^{ij}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} \\ &\quad + u^j u^l \int f^{(0)}(\boldsymbol{\eta}) H^{ik}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} + u^j u^k \int f^{(0)}(\boldsymbol{\eta}) H^{il}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} \\ &\quad + \rho u^i u^j u^k u^l. \end{aligned} \tag{4.46}$$

Defining the first integral as,

$$\begin{aligned} I_1 &\equiv \int f^{(0)}(\boldsymbol{\eta}) H^{ijkl}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} \\ &= \int \eta^i \eta^j \eta^k \eta^l f^{(0)}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} - \delta^{kl} \int \eta^i \eta^j f^{(0)}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} - \delta^{jl} \int \eta^i \eta^k f^{(0)}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} \\ &\quad - \delta^{jk} \int \eta^i \eta^l f^{(0)}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} - \delta^{il} \int \eta^j \eta^k f^{(0)}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} - \delta^{ik} \int \eta^j \eta^l f^{(0)}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} \\ &\quad - \delta^{ij} \int \eta^k \eta^l f^{(0)}(\boldsymbol{\eta}) d^D\boldsymbol{\eta} + \rho \delta^{ijkl}. \end{aligned} \tag{4.47}$$

Then use Eq.(4.41) and calling the first integral as I_2,

$$I_1 = I_2 + \rho\left(1 - 2\bar{\theta}\right)\delta^{ijkl}. \tag{4.48}$$

where,

$$I_2 \equiv \int \frac{\eta^i\eta^j\eta^k\eta^l}{z^{-1}e^{\frac{\eta^2}{2\theta}} \pm 1} d^D\boldsymbol{\eta}. \tag{4.49}$$

Since the distribution function is even, the product $\eta^i\eta^j\eta^k\eta^l$ must be even too, so as we have a nonzero I_2. Therefore, we have two possibilities: all indexes are equal ($i = j = k = l$) or they are equal in pairs ($i = j \neq k = l$).

Case 1: All indexes are equal

As our problem is symmetrical in D-space, we can choose one direction that the result would be the same for the other directions. Choosing the first coordinate, in Eq.(4.26): $\eta^i = \eta^j = \eta^k = \eta^l = \eta\cos\phi_1$

$$\begin{aligned} I_2^{(1)} &= \int_{\phi_{D-1}=0}^{2\pi}\int_{\phi_{D-2}=0}^{\pi}\cdots\int_{\phi_2}^{\pi}\int_{\phi_1=0}^{\pi}\sin^{D-2}\phi_1\sin^{D-3}\phi_2\ldots\sin^2\phi_{D-3}\sin\phi_{D-2} \\ &\quad \cdot d\phi_1\, d\phi_2\ldots d\phi_{D-1}\int_0^{\infty}\frac{\eta^4\cos^4\phi_1}{z^{-1}e^{\frac{\eta^2}{2\theta}}\pm 1}\eta^{D-1}d\eta \\ &= C_2\int_0^{\infty}\frac{\eta^{D+3}d\eta}{z^{-1}e^{\frac{\eta^2}{2\theta}}\pm 1}, \end{aligned} \tag{4.50}$$

where the index 1 in $I_2^{(1)}$ indicates that we re considering the case 1 and

$$\begin{aligned} C_2 \equiv{}& \int_{\phi_{D-1}=0}^{2\pi}\int_{\phi_{D-2}=0}^{\pi}\cdots\int_{\phi_2}^{\pi}\int_{\phi_1=0}^{\pi}\sin^{D-2}\phi_1\cos^4\phi_1\sin^{D-3}\phi_2\ldots\sin^2\phi_{D-3}\sin\phi_{D-2} \\ &.d\phi_1\, d\phi_2\ldots d\phi_{D-1}. \end{aligned} \tag{4.51}$$

Solving the integral in ϕ_1 separately

$$\int_0^{\pi}\sin^{D-2}\phi_1\cos^4\phi_1 d\phi_1 = \frac{\sin^{D-1}\phi_1\cos^3\phi_1}{D+2}\bigg|_0^{\pi} + \frac{3}{D+2}\int_0^{\pi}\sin^{D-2}\phi_1\cos^2\phi_1 d\phi_1,$$

where was used the following relation

$$\int \sin^n u\cos^m u\, du = \frac{\sin^{n+1}u\cos^{m-1}u}{n+m} + \frac{m-1}{n+m}\int\sin^n u\cos^{m-2}u\, du, \tag{4.52}$$

the first term is zero due to integration limits. Using (4.52) again

$$\begin{aligned}\int_0^\pi \sin^{D-2}\phi_1 \cos^4\phi_1 d\phi_1 &= \frac{3}{D+2}\frac{\sin^{D-1}\phi_1\cos\phi_1}{D}\Big|_0^\pi + \frac{3}{D(D+2)}\int_0^\pi \sin^{D-2}\phi_1 d\phi_1 \\ &= \frac{3}{D(D+2)}\int_0^\pi \sin^{D-2}\phi_1 d\phi_1. \end{aligned} \tag{4.53}$$

Substituting in (4.51)

$$\begin{aligned}C_2 = \frac{3}{D(D+2)}&\int_{\phi_{D-1}=0}^{2\pi}\int_{\phi_{D-2}=0}^{\pi}\cdots\int_{\phi_2}\int_{\phi_1=0}^{\pi}\sin^{D-2}\phi_1\sin^{D-3}\phi_2\ldots\sin^2\phi_{D-3}\sin\phi_{D-2} \\ &d\phi_1\, d\phi_2\ldots d\phi_{D-2}\, d\phi_{D-1},\end{aligned} \tag{4.54}$$

the integral is exactly the same as the definition of C_1 in eq. (4.33). Using (4.36) and the property of gamma functions $\Gamma(z+1) = z\Gamma(z)$

$$C_2 = \frac{3\pi^{\frac{D}{2}}}{2\Gamma\left(\frac{D}{2}+2\right)}. \tag{4.55}$$

Returning to eq. (4.50), we have

$$I_2^{(1)} = \frac{3}{4}\pi^{\frac{D}{2}}(2\theta)^{\frac{D+4}{2}} g_{\frac{D}{2}+2}(z). \tag{4.56}$$

Introducing $\rho = (2\pi)^{\frac{D}{2}}\theta^{\frac{D}{2}} g_{\frac{D}{2}}(z)$

$$I_2^{(1)} = 3\rho\theta^2 \frac{g_{\frac{D}{2}+2}(z)}{g_{\frac{D}{2}}(z)}. \tag{4.57}$$

Case 2: The indexes are equal in pairs

As before we choose any two directions because all of then are equivalent. Lets use (4.26) and (4.27) so that $\eta^i = \eta^j = \eta\cos\phi_1$ and $\eta^k = \eta^l = \eta\sin\phi_1\cos\phi_2$

$$\begin{aligned}I_2^{(2)} &= \int_{\phi_{D-1}=0}^{2\pi}\int_{\phi_{D-2}=0}^{\pi}\cdots\int_{\phi_2}\int_{\phi_1=0}^{\pi}\sin^{D-2}\phi_1\sin^{D-3}\phi_2\ldots\sin^2\phi_{D-3}\sin\phi_{D-2} \\ &\quad\cdot d\phi_1\, d\phi_2\ldots d\phi_{D-1}\int_0^\infty \frac{\eta^4\cos^2\phi_1\sin^2\phi_1\cos^2\phi_2\eta^{D-1}d\eta}{z^{-1}e^{\frac{\eta^2}{2\theta}}\pm 1} \\ &= C_3\int_0^\infty \frac{\eta^{D+3}d\eta}{z^{-1}e^{\frac{\eta^2}{2\theta}}\pm 1},\end{aligned} \tag{4.58}$$

where

$$C_3 = \int_{\phi_{D-1}=0}^{2\pi}\int_{\phi_{D-2}=0}^{\pi}\ldots\int_{\phi_2}^{\pi}\int_{\phi_1=0}^{\pi}\sin^D\phi_1\cos^2\phi_1\sin^{D-3}\phi_2\cos^2\phi_2\ldots\sin^2\phi_{D-3}\sin\phi_{D-2}\, d\phi_1\, d\phi_2\ldots d\phi_{D-2}\, d\phi_{D-1}. \quad (4.59)$$

Solving first the integral for ϕ_1,

$$\begin{aligned}\int_0^{\pi}\sin^D\phi_1\cos^2\phi_1 d\phi_1 &= \frac{\sin^{D+1}\phi_1\cos\phi_1}{D+2}\Big|_0^{\pi} + \frac{1}{D+2}\int_0^{\pi}\sin^D\phi_1 d\phi_1 \\ &= \frac{1}{D+2}\left[-\frac{1}{D}\sin^{D-1}\phi_1\Big|_0^{\pi} + \frac{D-1}{D}\int_0^{\pi}\sin^{D-2}\phi_1 d\phi_1\right] \\ &= \frac{D-1}{D(D+2)}\int_0^{\pi}\sin^{D-2}\phi_1 d\phi_1. \end{aligned} \quad (4.60)$$

I've used (4.52) and the following relation

$$\int\sin^n u\, du = -\frac{1}{n}\sin^{n-1}u\cos u + \frac{n-1}{n}\int\sin^{n-2}u\, du. \quad (4.61)$$

And the integral for ϕ_2 is

$$\begin{aligned}\int_0^{\pi}\sin^{D-3}\phi_2\cos^2\phi_2 d\phi_2 &= \frac{\sin^{D-2}\phi_2\cos\phi_2}{n-1}\Big|_0^{\pi} + \frac{1}{D-1}\int_0^{\pi}\sin^{D-3}\phi_2 d\phi_2 \\ &= \frac{1}{D-1}\int_0^{\pi}\sin^{D-3}\phi_2 d\phi_2. \end{aligned} \quad (4.62)$$

Putting (4.60) and (4.62) in Eq. (4.59)

$$\begin{aligned} C_3 &= \frac{1}{n(n+2)}\int_{\phi_{D-1}=0}^{2\pi}\int_{\phi_{D-2}=0}^{\pi}\ldots\int_{\phi_2}^{\pi}\int_{\phi_1=0}^{\pi}\sin^{D-2}\phi_1\sin^{D-3}\phi_2\ldots\sin^2\phi_{D-3}\sin\phi_{D-2} \\ &\quad \cdot d\phi_1\, d\phi_2\ldots d\phi_{D-2}\, d\phi_{D-1} \\ &= \frac{\pi^{\frac{D}{2}}}{2\Gamma\left(\frac{D}{2}+2\right)}. \end{aligned} \quad (4.63)$$

Therefore

$$I_2^{(2)} = \frac{\pi^{\frac{D}{2}}}{4}(2\pi)^{\frac{D+4}{2}}g_{\frac{D}{2}+2}(z) = \rho\theta^2\frac{g_{\frac{D}{2}+2}(z)}{g_{\frac{D}{2}}(z)}. \quad (4.64)$$

Comparing (4.57) and (4.64) see that $I_2^{(1)} = 3I_2^{(2)}$. So, we can summarize

$$I_2 = \int\frac{\eta^i\eta^j\eta^k\eta^l}{z^{-1}e^{\frac{\eta^2}{2\theta}}\pm 1}d^D\eta = \rho\theta^2\frac{g_{\frac{D}{2}+2}(z)}{g_{\frac{D}{2}}(z)}\delta^{ijkl}. \quad (4.65)$$

Substituting I_2 in (4.48)

$$I_1 = \rho \left[\theta^2 \frac{g_{\frac{D}{2}+2}(z)}{g_{\frac{D}{2}}(z)} - 2\theta \frac{g_{\frac{D}{2}+1}(z)}{g_{\frac{D}{2}}(z)} + 1 \right] \delta^{ijkl}. \tag{4.66}$$

We stress that only the $N = 4$ coefficient contains contributions proportional to θ^2. Thus an expansion of the BE-FD function limited to the $N = 3$ coefficient has the temperature only inside the pseudo temperature. At this point we introduce the notation defined in Eq.(4.142) which brings the function $g(z)$ of Eq.(4.76) into the $N = 4$ coefficient,

$$I_1 = \rho \left(\bar{\theta}^2 g(z) - 2\bar{\theta} + 1 \right) \delta^{ijkl}. \tag{4.67}$$

Finally, we obtain that the fourth coefficient,

$$\begin{aligned} a^{ijkl} &= \rho \left(\bar{\theta}^2 g(z) - 2\bar{\theta} + 1 \right) \delta^{ijkl} + \rho\bar{\theta} \left(u^i u^j \delta^{kl} + u^i u^k \delta^{jl} + u^i u^l \delta^{jk} \right. \\ &\quad \left. + u^k u^l \delta^{ij} + u^j u^l \delta^{ik} + u^j u^k \delta^{il} \right) + \rho u^i u^j u^k u^l. \end{aligned} \tag{4.68}$$

In power of the four Hermite coefficients we write their contractions to the Hermite polynomials themselves,

$$aH = \rho \tag{4.69}$$

$$a^i H^i = \rho(\boldsymbol{\xi} \cdot \boldsymbol{u}) \tag{4.70}$$

$$a^{ij} H^{ij} = \rho \big[\big(\bar{\theta} - 1 \big) (\boldsymbol{\xi}^2 - D) + (\boldsymbol{\xi} \cdot \boldsymbol{u})^2 - \boldsymbol{u}^2 \big] \tag{4.71}$$

$$\begin{aligned} a^{ijk} H^{ijk} &= \rho \{ (\boldsymbol{\xi} \cdot \boldsymbol{u})^3 - 3\boldsymbol{u}^2 (\boldsymbol{\xi} \cdot \boldsymbol{u}) + \big(\bar{\theta} - 1 \big) \\ &\quad \cdot \big[3(\boldsymbol{\xi} \cdot \boldsymbol{u}) \boldsymbol{\xi}^2 - 3(\boldsymbol{\xi} \cdot \boldsymbol{u}) D - 6 \big(\boldsymbol{\xi} \cdot \boldsymbol{u} \big) \big] \} \end{aligned} \tag{4.72}$$

$$\begin{aligned} a^{ijkl} H^{ijkl} &= \rho \{ \big[\bar{\theta}^2 g(z) - 2\bar{\theta} + 1 \big] \\ &\quad \cdot \big(3\boldsymbol{\xi}^4 - 6D\boldsymbol{\xi}^2 - 12\boldsymbol{\xi}^2 + 3D^2 + 6D \big) + 6 \big(\bar{\theta} - 1 \big) \\ &\quad \cdot \big[(\boldsymbol{\xi} \cdot \boldsymbol{u})^2 (\boldsymbol{\xi}^2 - D - 4) + \boldsymbol{u}^2 \big(D + 2 - \boldsymbol{\xi}^2 \big) \big] \\ &\quad + \big[(\boldsymbol{\xi} \cdot \boldsymbol{u})^4 - 6(\boldsymbol{\xi} \cdot \boldsymbol{u})^2 \boldsymbol{u}^2 + 3\boldsymbol{u}^4 \big] \}. \end{aligned} \tag{4.73}$$

From Eqs.(4.22) and (A.2), one obtains that,

$$f^{(0)}(\boldsymbol{x},\boldsymbol{\xi}) = \omega(\boldsymbol{\xi})\left(aH + a^i H^i + \frac{1}{2!}a^{ij}H^{ij} + \frac{1}{3!}a^{ijk}H^{ijk} + \frac{1}{4!}a^{ijkl}H^{ijkl}\right). \tag{4.74}$$

Therefore the BE-FD function expanded in Hermite polynomials until the fourth order is,

$$\begin{aligned} f^{(0)}(\boldsymbol{x},\boldsymbol{\xi}) &= \omega(\boldsymbol{\xi})\rho\Bigg\{1 + (\boldsymbol{\xi}\cdot\boldsymbol{u})\left(1 - \frac{1}{2}\boldsymbol{u}^2\right) + (\boldsymbol{\xi}\cdot\boldsymbol{u})^2\left(\frac{1}{2}\right. \\ &\quad \left. -\frac{1}{4}\boldsymbol{u}^2\right) + \frac{1}{6}(\boldsymbol{\xi}\cdot\boldsymbol{u})^3 - \frac{1}{2}\boldsymbol{u}^2 + \frac{1}{8}\boldsymbol{u}^4 + \frac{1}{24}(\boldsymbol{\xi}\cdot\boldsymbol{u})^4 \\ &\quad + \left(\bar{\theta} - 1\right)\cdot\left[\frac{1}{2}(\boldsymbol{\xi}^2 - D) + \frac{1}{2}(\boldsymbol{\xi}\cdot\boldsymbol{u})(\boldsymbol{\xi}^2 - D - 2)\right. \\ &\quad \left. + \frac{1}{4}(\boldsymbol{\xi}\cdot\boldsymbol{u})^2(\boldsymbol{\xi}^2 - D - 4) + \frac{1}{4}\boldsymbol{u}^2(D + 2 - \boldsymbol{\xi}^2)\right] \\ &\quad + \frac{1}{8}\left[\bar{\theta}^2 g(z) - 2\bar{\theta} + 1\right]\left[\boldsymbol{\xi}^4 + (D+2)(D - 2\boldsymbol{\xi}^2)\right]\Bigg\}, \end{aligned} \tag{4.75}$$

where the definition of ρ, $\bar{\theta}$, and $g(z)$, are given in Eqs.(4.4), (4.2) and

$$g(z) \equiv \frac{g_{\frac{D}{2}}(z)\cdot g_{\frac{D}{2}+2}(z)}{\left(g_{\frac{D}{2}+1}(z)\right)^2}, \tag{4.76}$$

respectively. In the section 3.2 we Taylor expanded the MB distribution function thus providing an independent check that BE-FD and MB coincide in the limit that $g_\nu(z) \to z$. Analogously to Eq.3.71, the equilibrium distribution function in discrete space is

$$\begin{aligned} f_\alpha^{(0)} &= w_\alpha\rho\Bigg\{1 + (\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})\left(1 - \frac{1}{2}\boldsymbol{u}^2\right) + \frac{1}{6}(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})^3 + (\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})^2\left(\frac{1}{2} - \frac{1}{4}\boldsymbol{u}^2\right) - \frac{1}{2}\boldsymbol{u}^2 \\ &\quad + \frac{1}{8}\boldsymbol{u}^4 + \frac{1}{24}(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})^4 + \left(\bar{\theta} - 1\right)\cdot\left[\frac{1}{2}(\boldsymbol{\xi}_\alpha^2 - D) + \frac{1}{2}(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})(\boldsymbol{\xi}_\alpha^2 - D - 2)\right. \\ &\quad \left. + \frac{1}{4}(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})^2(\boldsymbol{\xi}_\alpha^2 - D - 4) + \frac{1}{4}\boldsymbol{u}^2(D + 2 - \boldsymbol{\xi}_\alpha^2)\right] + \frac{1}{8}\left[\bar{\theta}^2 g(z) - 2\bar{\theta} + 1\right] \\ &\quad \cdot[\boldsymbol{\xi}_\alpha^4 + (D+2)(D - 2\boldsymbol{\xi}_\alpha^2)]\Bigg\}. \end{aligned} \tag{4.77}$$

Thus the continuum and discrete distribution functions basically differ by the replacement of the gaussian function $\omega(\boldsymbol{\xi})$ by the weights w_α.

4.2 Multi-scale expansion

In this section we perform the Chapman-Enskog analysis of the $N = 4$ order BGK-Boltzmann theory and obtain the macroscopic hydrodynamical equations. The local density, macroscopic velocity and energy are obtained at any time and at any grid point through the definitions:

$$\rho(\boldsymbol{x}, t) = \sum_{\alpha} f_{\alpha}(\boldsymbol{x}, t) \tag{4.78}$$

$$\boldsymbol{u}(\boldsymbol{x}, t) = \frac{1}{\rho(\boldsymbol{x}, t)} \sum_{\alpha} \boldsymbol{\xi} f_{\alpha}(\boldsymbol{x}, t) \tag{4.79}$$

$$\frac{D}{2}\bar{\theta}(\boldsymbol{x}, \boldsymbol{t}) = \frac{1}{\rho(\boldsymbol{x}, t)} \sum_{\alpha} \frac{\left[\boldsymbol{\xi}_{\alpha} - \boldsymbol{u}(\boldsymbol{x})\right]^2}{2} f_{\alpha}(\boldsymbol{x}, t). \tag{4.80}$$

The last expression truly defines $\bar{\theta}$ and can be expressed as,

$$\frac{D}{2}\bar{\theta}(\boldsymbol{x}, \boldsymbol{t}) + \frac{1}{2}\boldsymbol{u}(\boldsymbol{x}, t)^2 = \frac{1}{\rho(\boldsymbol{x}, t)} \sum_{\alpha} \frac{\boldsymbol{\xi}_{\alpha}^2}{2} f_{\alpha}(\boldsymbol{x}, t). \tag{4.81}$$

The Chapman-Enskog relations (see Eqs.(3.25), (3.26) and (3.27)) must hold to assure the macroscopic thermodynamic equations [35, 41]:

$$\sum_{\alpha} f_{\alpha} = \sum_{\alpha} f_{\alpha}^{(0)} \tag{4.82}$$

$$\sum_{\alpha} f_{\alpha} \boldsymbol{\xi}_{\boldsymbol{\alpha}} = \sum_{\alpha} f_{\alpha}^{(0)} \boldsymbol{\xi}_{\boldsymbol{\alpha}} \tag{4.83}$$

$$\sum_{\alpha} f_{\alpha} \boldsymbol{\xi}_{\alpha}^2 = \sum_{\alpha} f_{\alpha}^{(0)} \boldsymbol{\xi}_{\alpha}^2. \tag{4.84}$$

These equations imply that $\rho = \sum_{\alpha} f_{\alpha}^{(0)}$, $\rho\boldsymbol{u} = \sum_{\alpha} \boldsymbol{\xi} f_{\alpha}^{(0)}$, and $D\rho\bar{\theta}/2 + \rho\boldsymbol{u}^2/2 = \sum_{\alpha} \boldsymbol{\xi}_{\alpha}^2 f_{\alpha}^{(0)}/2$. The quantities ρ, $\boldsymbol{u}$, and θ, obtained from Eqs.(4.78), (4.79) and (4.80), respectively, must be fed back into $f_{\alpha}^{(0)}$, which, by its turn, sets the evolution to a new $f_{\alpha}(\boldsymbol{x}, t)$, according

to Eq.(3.72). Next we seek a formal solution of the distribution f_α in terms of $f_\alpha^{(0)}$. To obtain this solution two key ingredients must be considered. Firstly we Taylor expand f_α until second order in the time step:

$$f_\alpha(\boldsymbol{x}+\boldsymbol{\xi_\alpha}\Delta t, t+\Delta t) \cong f_\alpha(\boldsymbol{x},t) + \Delta t\left[\xi_\alpha^i \frac{\partial f_\alpha}{\partial x^i} + \frac{\partial f_\alpha}{\partial t}\right] + \frac{(\Delta t)^2}{2}\left[\frac{\partial^2 f_\alpha}{\partial t^2} + \xi_\alpha^i\xi_\alpha^j\frac{\partial^2 f_\alpha}{\partial x^i \partial x^j} + 2\xi_\alpha^i \frac{\partial^2 f_\alpha}{\partial x^i \partial t}\right]. \tag{4.85}$$

Then the discrete Boltzmann equation, Eq.(3.24), becomes in this approximation,

$$\xi_\alpha^i \frac{\partial f_\alpha}{\partial x^i} + \frac{\partial f_\alpha}{\partial t} + \frac{\Delta t}{2}\left[\frac{\partial^2 f_\alpha}{\partial t^2} + \xi_\alpha^i\xi_\alpha^j\frac{\partial^2 f_\alpha}{\partial x^i \partial x^j} + 2\xi_\alpha^i \frac{\partial^2 f_\alpha}{\partial x^i \partial t}\right] \cong -\frac{1}{\tau}\left(f_\alpha - f_\alpha^{(0)}\right). \tag{4.86}$$

Secondly we introduce the *Chapman-Enskog expansion*, which means to expand the distribution function in terms of a parameter ϵ that represents the Knudsen's number (ratio between the mean free path and a representative physical length scale)

$$f_\alpha = f_\alpha^{(0)} + \epsilon f_\alpha^{(1)} + \epsilon^2 f_\alpha^{(2)} + ... \tag{4.87}$$

Notice that because of the Chapman-Enskog relations, Eqs.(4.82), (4.83) and (4.84), the ϵ dependent terms must satisfy the following relations:

$$\sum_\alpha f_\alpha^{(1)} = \sum_\alpha f_\alpha^{(2)} = 0, \tag{4.88}$$

$$\sum_\alpha \boldsymbol{\xi}_\alpha f_\alpha^{(1)} = \sum_\alpha \boldsymbol{\xi}_\alpha f_\alpha^{(2)} = 0, \tag{4.89}$$

$$\sum_\alpha \boldsymbol{\xi}_\alpha^2 f_\alpha^{(1)} = \sum_\alpha \boldsymbol{\xi}_\alpha^2 f_\alpha^{(2)} = 0. \tag{4.90}$$

The parameter ϵ also sets the scale for the derivatives of time and space that are expanded in Eq.(4.87):

$$\frac{\partial}{\partial t} = \epsilon\frac{\partial}{\partial t_1} + \epsilon^2\frac{\partial}{\partial t_2}, \tag{4.91}$$

$$\frac{\partial}{\partial x^i} = \epsilon\frac{\partial}{\partial x_1^i}. \tag{4.92}$$

We stress for later purposes that the cross time and position derivative is given by,

$$\frac{\partial}{\partial x^i}\frac{\partial}{\partial t} = \epsilon^2 \frac{\partial}{\partial t_1}\frac{\partial}{\partial x_1^i}, \tag{4.93}$$

to the studied order ϵ^2. Applying (4.87), (4.91) and (4.92) in (4.86),

$$\epsilon\left[\xi_\alpha^i \frac{\partial f_\alpha^{(0)}}{\partial x_1^i} + \frac{\partial f_\alpha^{(0)}}{\partial t_1}\right] + \epsilon^2\left[\xi_\alpha^i \frac{\partial f_\alpha^{(1)}}{\partial x_1^i} + \frac{\partial f_\alpha^{(1)}}{\partial t_1} + \frac{\partial f_\alpha^{(0)}}{\partial t_2} + \frac{\Delta t}{2}\frac{\partial^2 f_\alpha^{(0)}}{\partial t_1^2} + \frac{\Delta t}{2}\xi_\alpha^i \xi_\alpha^j \frac{\partial^2 f_\alpha^{(0)}}{\partial x_1^i \partial x_1^j}$$
$$+\Delta t \xi_\alpha^i \frac{\partial^2 f_\alpha^{(0)}}{\partial x_1^i \partial t_1}\right] = -\frac{1}{\tau}[\epsilon f_\alpha^{(1)} + \epsilon^2 f_\alpha^{(2)} + ...]. \tag{4.94}$$

Next we collect the terms of same order, and the first order terms give that,

$$-\frac{1}{\tau} f_\alpha^{(1)} = \left[\xi_\alpha^i \frac{\partial f_\alpha^{(0)}}{\partial x_1^i} + \frac{\partial f_\alpha^{(0)}}{\partial t_1}\right]. \tag{4.95}$$

For second order one obtains that,

$$-\frac{1}{\tau} f_\alpha^{(2)} = \xi_\alpha^i \frac{\partial f_\alpha^{(1)}}{\partial x_1^i} + \frac{f_\alpha^{(1)}}{\partial t_1} + \frac{\partial f_\alpha^{(0)}}{\partial t_2} + \frac{\Delta t}{2}\frac{\partial^2 f_\alpha^{(0)}}{\partial t_1^2} + \frac{\Delta t}{2}\xi_\alpha^i \xi_\alpha^j \frac{\partial^2 f_\alpha^{(0)}}{\partial x_1^i \partial x_1^j} + \Delta t \xi_\alpha^i \frac{\partial^2 f_\alpha^{(0)}}{\partial x_1^i \partial t_1}. \tag{4.96}$$

We derive Eq.(4.95) with respect to t_1 and x_1^i to find that Eq.(4.96) becomes,

$$-\frac{1}{\tau} f_\alpha^{(2)} = \frac{\partial f_\alpha^{(0)}}{\partial t_2} + \left(1 - \frac{\Delta t}{2\tau}\right)\left[\frac{\partial f_\alpha^{(1)}}{\partial t_1} + \xi_\alpha^i \frac{\partial f_\alpha^{(1)}}{\partial x_1^i}\right]. \tag{4.97}$$

In summary we found a solution for the discrete Boltzmann (Eq.(4.86)), which is the distribution f_α, given by Eq.(4.87), as a function of $f_\alpha^{(0)}$ and its derivatives through Eqs.(4.95) and (4.97). It remains to reconstruct the time and the position, which are defined by Eqs.(4.91) and (4.92). This will be done separately for the mass, momentum and energy.

4.2.1 Conservation of mass

To obtain the continuity equation, one must sum over all directions α in Eq.(4.95),

$$\frac{1}{\tau}\sum_\alpha f_\alpha^{(1)} = -\frac{\partial}{\partial t_1}\sum_\alpha f_\alpha^{(0)} - \frac{\partial}{\partial x_1^i}\sum_\alpha f_\alpha^0 \xi_\alpha^i. \tag{4.98}$$

Recall the definitions of ρ, $\boldsymbol{u}$, Eqs.(4.78) and (4.79), and the Chapman-Enskog relations of Eqs.(4.82) and (4.83):

$$\frac{\partial \rho}{\partial t_1} + \frac{\partial}{\partial x_1^i}(\rho u^i) = 0. \tag{4.99}$$

This is not yet the continuity equation as the time derivative is over t_1 instead of t. To fix it, sum over α in Eq.(4.97):

$$-\frac{1}{\tau}\sum_\alpha f_\alpha^{(2)} = \frac{\partial}{\partial t_2}\sum_\alpha f_\alpha^{(0)} + \left(1 - \frac{\Delta t}{2\tau}\right)\left[\frac{\partial}{\partial t_1}\sum_\alpha f_\alpha^{(1)} + \sum_\alpha \xi_\alpha^i \frac{\partial f_\alpha^{(1)}}{\partial x_1^i}\right]. \tag{4.100}$$

The above equation is no more than,

$$\frac{\partial \rho}{\partial t_2} = 0. \tag{4.101}$$

To reconstruct the time and space derivative, take Eqs.(4.91) and (4.92) applied to the density, respectively,

$$\frac{\partial \rho}{\partial t} = \epsilon \frac{\partial \rho}{\partial t_1} + \epsilon^2 \frac{\partial \rho}{\partial t_2} = \epsilon \frac{\partial \rho}{\partial t_1} \tag{4.102}$$

$$\frac{\partial \rho}{\partial x^i} = \epsilon \frac{\partial \rho}{\partial x_1^i}. \tag{4.103}$$

Then the quantum continuity equation,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x^i}(\rho u^i) = 0, \tag{4.104}$$

is obtained. Remember that the quantum density is defined as in Eq.(4.4)

4.2.2 Conservation of momentum

The derivation of the conservation of momentum equation follows similar steps, which means that Eqs.(4.95) and (4.97) are multiplied by ξ_α^i and next summed over α.

$$-\frac{1}{\tau}\sum_\alpha \xi_\alpha^i f_\alpha^{(1)} = \frac{\partial}{\partial x_1^j}\sum_\alpha \xi_\alpha^i \xi_\alpha^j f_\alpha^{(0)} + \frac{\partial}{\partial t_1}\sum_\alpha \xi_\alpha^i f_\alpha^{(0)}. \tag{4.105}$$

Using the Chapman-Enskog relation of Eq.(4.83), it follows that,

$$\frac{\partial}{\partial t_1}\sum_\alpha \xi_\alpha^i f_\alpha^{(0)} + \frac{\partial}{\partial x_1^j}\sum_\alpha \xi_\alpha^i \xi_\alpha^j f_\alpha^{(0)} = 0. \tag{4.106}$$

Next from Eq.(4.97) one obtains that,

$$-\frac{1}{\tau}\sum_{\alpha}\xi_{\alpha}^{i}f_{\alpha}^{(2)}=\frac{\partial}{\partial t_{2}}\sum_{\alpha}\xi_{\alpha}^{i}f_{\alpha}^{(0)}+\left(1-\frac{\Delta t}{2\tau}\right)\left[\frac{\partial}{\partial t_{1}}\sum_{\alpha}\xi_{\alpha}^{i}f_{\alpha}^{(1)}+\frac{\partial}{\partial x_{1}^{j}}\sum_{\alpha}\xi_{\alpha}^{i}\xi_{\alpha}^{j}f_{\alpha}^{(1)}\right] \quad (4.107)$$

We apply Eq.(4.89) twice in the above equation to obtain that,

$$\frac{\partial}{\partial t_{2}}\sum_{\alpha}\xi_{\alpha}^{i}f_{\alpha}^{(0)}+\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x_{1}^{j}}\sum_{\alpha}\xi_{\alpha}^{i}\xi_{\alpha}^{j}f_{\alpha}^{(1)}=0. \quad (4.108)$$

Next consider the construction ϵ times Eq.(4.106) plus ϵ^2 times Eq.(4.108):

$$\left(\epsilon\frac{\partial}{\partial t_{1}}+\epsilon^{2}\frac{\partial}{\partial t_{2}}\right)\sum_{\alpha}\xi_{\alpha}^{i}f_{\alpha}^{(0)}+\epsilon\frac{\partial}{\partial x_{1}^{j}}\sum_{\alpha}\xi_{\alpha}^{i}\xi_{\alpha}^{j}f_{\alpha}^{(0)}$$
$$+\epsilon^{2}\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x_{1}^{j}}\sum_{\alpha}\xi_{\alpha}^{i}\xi_{\alpha}^{j}f_{\alpha}^{(1)}=0. \quad (4.109)$$

We use Eqs.(4.79), (4.83) and introduce Eq.(4.95) into the above equation to write it solely in terms of moments of $f_{\alpha}^{(0)}$:

$$\left(\epsilon\frac{\partial}{\partial t_{1}}+\epsilon^{2}\frac{\partial}{\partial t_{2}}\right)(\rho u^{i})+\epsilon\frac{\partial}{\partial x_{1}^{j}}\sum_{\alpha}\xi_{\alpha}^{i}\xi_{\alpha}^{j}f_{\alpha}^{(0)}-\tau\epsilon^{2}\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x_{1}^{j}}\frac{\partial}{\partial x_{1}^{k}}\sum_{\alpha}\xi_{\alpha}^{i}\xi_{\alpha}^{j}\xi_{\alpha}^{k}f_{\alpha}^{(0)}$$
$$-\tau\epsilon^{2}\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x_{1}^{j}}\frac{\partial}{\partial t_{1}}\sum_{\alpha}\xi_{\alpha}^{i}\xi_{\alpha}^{j}f_{\alpha}^{(0)}=0. \quad (4.110)$$

The true time and position derivatives are given by Eqs.(4.91), (4.92) and (4.93), and the above equation acquires the form,

$$\frac{\partial}{\partial t}(\rho u^{i})+\frac{\partial}{\partial x^{j}}\pi^{ij}-\tau\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x^{j}}\frac{\partial}{\partial x^{k}}\pi^{ijk}-\tau\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x^{i}}\frac{\partial}{\partial t}\pi^{ij}=0, \quad (4.111)$$

by definition of $\pi^{ij}\equiv\sum_{\alpha}\xi_{\alpha}^{i}\xi_{\alpha}^{j}f_{\alpha}^{(0)}$, $\pi^{ijk}\equiv\sum_{\alpha}\xi_{\alpha}^{i}\xi_{\alpha}^{j}\xi_{\alpha}^{k}f_{\alpha}^{(0)}$. We call it the *master equation for the conservation of momentum*. To determine the tensors π^{ij} and π^{ijk} in terms of the macroscopic quantities one must introduce $f_{\alpha}^{(0)}$ given by Eq.(4.77).

To accomplish such task one must invoke some relations calculated in appendix D. These are Eqs.(D.1), (D.2), (D.3), (D.4) and (D.5) to calculate π^{ij} and Eqs.(D.6), (D.7) and (D.8) to derive π^{ijk}. After some algebra we find that,

$$\pi^{ij}=\rho\left(\bar{\theta}\delta^{ij}+u^{i}u^{j}\right) \quad (4.112)$$
$$\pi^{ijk}=\rho\left[\bar{\theta}\left(u^{k}\delta^{ij}+u^{j}\delta^{ik}+u^{i}\delta^{jk}\right)+u^{i}u^{j}u^{k}\right].$$

Substituting these results in Eq.(4.111), we find that the equation for the momentum conservation is,

$$\frac{\partial}{\partial t}\left(\rho u^i\right)+\frac{\partial}{\partial x^j}\left[\rho\left(\bar{\theta}\delta^{ij}+u^iu^j\right)\right]-\tau\left(1-\frac{\Delta t}{2\tau}\right)\cdot\frac{\partial}{\partial x^j}\frac{\partial}{\partial x^k}\left\{\rho\left[\bar{\theta}\left(u^k\delta^{ij}+u^j\delta^{ik}\right.\right.\right.$$
$$\left.\left.\left.+u^i\delta^{jk}\right)+u^iu^ju^k\right]\right\}-\tau\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x^i}\frac{\partial}{\partial t}\left[\rho\left(\bar{\theta}\delta^{ij}+u^iu^j\right)\right]=0. \tag{4.113}$$

Notice that in the above equation the temperature is only present through the pseudo temperature. The last step is to replace the cross derivative term $\partial^2/\partial t\partial x^k$ by a positional derivative term, $\partial^2/\partial x^i\partial x^j$. This task is carried in the section 4.2.4 and leads to the momentum equation of Eq.(4.134).

4.2.3 Conservation of energy

The derivation of the conservation of energy equation also follows from Eqs.(4.95) and (4.97), but in this case multiplied by $\boldsymbol{\xi}_\alpha^2$ instead, and summed over α.

$$-\frac{1}{\tau}\sum_\alpha f_\alpha^{(1)}\boldsymbol{\xi}_\alpha^2=\sum_\alpha\boldsymbol{\xi}_\alpha^2\xi_\alpha^j\frac{\partial f_\alpha^{(0)}}{\partial x_1^j}+\sum_\alpha\boldsymbol{\xi}_\alpha^2\frac{\partial f_\alpha^{(0)}}{\partial t_1}. \tag{4.114}$$

The Chapman-Enskog relation of Eq.(4.84) renders the left side of the above equation equal to zero, and so,

$$\frac{\partial}{\partial t_1}\sum_\alpha\boldsymbol{\xi}_\alpha^2f_\alpha^{(0)}+\frac{\partial}{\partial x_1^j}\sum_\alpha\boldsymbol{\xi}_\alpha^2\xi_\alpha^jf_\alpha^{(0)}=0. \tag{4.115}$$

Similarly Eq.(4.97) leads to the following equation.

$$\begin{aligned}-\frac{1}{\tau}\sum_\alpha\boldsymbol{\xi}_\alpha^2f_\alpha^{(2)} &= \frac{\partial}{\partial t_2}\sum_\alpha\boldsymbol{\xi}_\alpha^2f_\alpha^{(0)}+\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial t_1}\sum_\alpha\boldsymbol{\xi}_\alpha^2f_\alpha^{(1)}\\ &\quad+\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x_1^j}\sum_\alpha\boldsymbol{\xi}_\alpha^2\xi_\alpha^jf_\alpha^{(1)}.\end{aligned} \tag{4.116}$$

The Chapman-Enskog relation of Eq.(4.84) renders two terms null, including the left side.

$$\frac{\partial}{\partial t_2}\sum_\alpha\boldsymbol{\xi}_\alpha^2f_\alpha^{(0)}+\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x_1^j}\sum_\alpha\boldsymbol{\xi}_\alpha^2\xi_\alpha^jf_\alpha^{(1)}=0. \tag{4.117}$$

To get the time and the position derivatives consider Eqs.(4.91) and (4.92), and so, take Eq.(4.115) times ϵ plus Eq. (4.117) times ϵ^2.

$$\left(\epsilon\frac{\partial}{\partial t_1}+\epsilon^2\frac{\partial}{\partial t_2}\right)\sum_\alpha \boldsymbol{\xi}_\alpha^2 f_\alpha^{(0)}+\epsilon\frac{\partial}{\partial x_1^j}\sum_\alpha \boldsymbol{\xi}_\alpha^2\xi_\alpha^j f_\alpha^{(0)}$$
$$+\epsilon^2\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x_1^j}\sum_\alpha \boldsymbol{\xi}_\alpha^2\xi_\alpha^j f_\alpha^{(1)}=0. \tag{4.118}$$

Introduce Eq.(4.81) and Eq.(4.95) to obtain that,

$$\left(\epsilon\frac{\partial}{\partial t_1}+\epsilon^2\frac{\partial}{\partial t_2}\right)\sum_\alpha \boldsymbol{\xi}_\alpha^2 f_\alpha^{(0)}+\epsilon\frac{\partial}{\partial x_1^j}\sum_\alpha \boldsymbol{\xi}_\alpha^2\xi_\alpha^j f_\alpha^{(0)}$$
$$-\tau\epsilon^2\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x_1^j}\frac{\partial}{\partial x_1^k}\sum_\alpha \boldsymbol{\xi}_\alpha^2\xi_\alpha^j\xi_\alpha^k f_\alpha^{(0)}$$
$$-\tau\epsilon^2\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x_1^j}\frac{\partial}{\partial t_1}\sum_\alpha \boldsymbol{\xi}_\alpha^2\xi_\alpha^j f_\alpha^{(0)}=0. \tag{4.119}$$

Then one gets,

$$\frac{\partial}{\partial t}\phi+\frac{\partial}{\partial x^j}\phi^j-\tau\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x^j}\frac{\partial}{\partial x^k}\phi^{jk}-\tau\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x^j}\frac{\partial}{\partial t}\phi^j=0. \tag{4.120}$$

This is the *master equation for the conservation of energy*. We define $\phi\equiv\sum_\alpha {\boldsymbol{\xi_\alpha}}^2 f_\alpha^{(0)}/2$, $\phi^j\equiv\sum_\alpha {\boldsymbol{\xi_\alpha}}^2\xi_\alpha^j f_\alpha^{(0)}/2$ and $\phi^{jk}\equiv\sum_\alpha {\boldsymbol{\xi_\alpha}}^2\xi_\alpha^j\xi_\alpha^k f_\alpha^{(0)}/2$ and use Eq.(4.93). It is straightforward to calculate ϕ, ϕ^j and ϕ^{jk} from the expressions developed in the appendix D. Then one determines these tensors in terms of the macroscopic quantities contained in $f_\alpha^{(0)}$, given by Eq.(4.77).

$$\phi=\frac{1}{2}\rho\boldsymbol{u}^2+\frac{D}{2}\rho\bar{\theta} \tag{4.121}$$

$$\phi^j=\frac{\rho}{2}\left[u^j\boldsymbol{u}^2+\bar{\theta}\,(D+2)\,u^j\right] \tag{4.122}$$

$$\phi^{jk}=\frac{\rho}{2}\left[\boldsymbol{u}^2u^ju^k+\bar{\theta}\,(D+4)\,u^ju^k+\bar{\theta}\boldsymbol{u}^2\delta^{jk}+\bar{\theta}^2g(z)\,(D+2)\,\delta^{jk}\right]. \tag{4.123}$$

Notice that among the above three tensors only ϕ^{jk} contains an explicit quadratic term in the temperature, which leads to the presence of the $g(z)$ function in Eq.(4.76). Thus

the energy equation cannot be purely expressed in terms of ρ, $\boldsymbol{u}$ and $\bar{\theta}$. I write it with a $g(z)-1$ term intentionally in its right side. The left side corresponds to the classical (MB) case, replacing $\bar{\theta}$ by θ,

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\frac{\rho}{2}\boldsymbol{u}^2+\frac{\rho}{2}D\bar{\theta}\right)+\frac{\partial}{\partial x^j}\left[\left(\frac{\rho}{2}\boldsymbol{u}^2+\frac{\rho}{2}\bar{\theta}(D+2)\right)u^j\right]\\
&-\tau\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x^j}\frac{\partial}{\partial x^k}\left[\frac{\rho}{2}\boldsymbol{u}^2u^ju^k\right.\\
&\left.+\frac{\rho}{2}\bar{\theta}(D+4)u^ju^k+\frac{\rho}{2}\bar{\theta}\boldsymbol{u}^2\delta^{jk}+\frac{\rho}{2}\bar{\theta}^2(D+2)\delta^{jk}\right]\\
&-\tau\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x^j}\frac{\partial}{\partial t}\left[\left(\frac{\rho}{2}\boldsymbol{u}^2+\frac{\rho}{2}\bar{\theta}(D+2)\right)u^j\right]\\
=\;&\tau\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial x^j}\frac{\partial}{\partial x^k}\left[\frac{\rho}{2}\bar{\theta}^2\left(g(z)-1\right)(D+2)\delta^{jk}\right].
\end{aligned}\tag{4.124}$$

Similarly to the momentum case, the cross derivative term $\partial^2/\partial t\partial x^k$ is replaced by a positional derivative term, $\partial^2/\partial x^i\partial x^j$, in the next section, and this leads to Eq.(4.140).

4.2.4 The position and time cross derivative terms of the momentum and energy conservation equations

In this section we seek replacement of the $\frac{\partial}{\partial x^j}\frac{\partial}{\partial t}$ terms contained in Eqs. (4.113) and (4.124) by position derivatives. The key to this step is to consider that terms proportional to the square of the collision time τ, namely, proportional to $[\tau(1-\Delta t/2\tau)]^2$, are neglected. Thus it consider the above equations in the limit $\tau\to 0$ and $\Delta t/\tau$ fixed. Setting $\tau=0$ in Eqs. (4.113) and (4.124) gives that,

$$\frac{\partial}{\partial t}\left(\rho u^i\right)+\frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\delta^{ij}+\rho u^iu^j\right)=0,\tag{4.125}$$

$$\frac{\partial}{\partial t}\left(\frac{\rho}{2}\boldsymbol{u}^2+\frac{\rho}{2}D\bar{\theta}\right)+\frac{\partial}{\partial x^j}\left[\left(\frac{\rho}{2}\boldsymbol{u}^2+\frac{\rho}{2}\bar{\theta}(D+2)\right)u^j\right]=0.\tag{4.126}$$

The momentum conservation equation

Introducing the continuity equation (4.104) into Eq. (4.125) gives,

$$\rho\frac{\partial u^i}{\partial t}+\frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\delta^{ij}\right)+\rho u^j\frac{\partial u^i}{\partial x^j}=0.\tag{4.127}$$

We will develop some identities from Eqs.(4.104) and, (4.127).

$$\begin{aligned}
&\frac{\partial}{\partial t}(\rho \boldsymbol{u}^2) = \boldsymbol{u}^2 \frac{\partial \rho}{\partial t} + 2\rho u^j \frac{\partial u^j}{\partial t} \\
= \; & -\boldsymbol{u}^2 \frac{\partial}{\partial x^j}(\rho u^j) - 2u^j \frac{\partial}{\partial x^i}\left(\rho\bar{\theta}\delta^{ij}\right) - u^j \frac{\partial}{\partial x^j}(\rho \boldsymbol{u}^2) \\
= \; & -\frac{\partial}{\partial x^j}(\rho \boldsymbol{u}^2 u^j) - 2u^j \frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\right). \qquad (4.128)
\end{aligned}$$

Introducing Eq.(4.128) into Eq.(4.126) gives the identity,

$$\frac{\partial}{\partial t}\left(\rho\bar{\theta}D\right) - 2u^j \frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\right) + \frac{\partial}{\partial x^j}\left[\rho\bar{\theta}(D+2)u^j\right] = 0,$$

that can be expressed as,

$$\frac{\partial}{\partial t}\left(\rho\bar{\theta}D\right) = -\frac{\partial}{\partial x^j}\left(\rho\bar{\theta}Du^j\right) - 2\rho\bar{\theta}\frac{\partial u^j}{\partial x^j}. \qquad (4.129)$$

Starting from,

$$\frac{\partial}{\partial t}(\rho u^i u^j) = u^i u^j \frac{\partial \rho}{\partial t} + \rho u^j \frac{\partial u^i}{\partial t} + \rho u^i \frac{\partial u^j}{\partial t}, \qquad (4.130)$$

and using the continuity equation, and Eq.(4.127), yields that,

$$\begin{aligned}
&\frac{\partial}{\partial t}(\rho u^i u^j) = -u^i u^j \frac{\partial}{\partial x^k}(\rho u^k) - u^k \frac{\partial}{\partial x^k}(u^i u^j)\rho - u^j \frac{\partial}{\partial x^i}\left(\rho\bar{\theta}\right) - u^i \frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\right) \\
= \; & -\frac{\partial}{\partial x^k}(\rho u^i u^j u^k) - u^j \frac{\partial}{\partial x^i}\left(\rho\bar{\theta}\right) - u^i \frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\right). \qquad (4.131)
\end{aligned}$$

Thus the temporal evolution,

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\rho\bar{\theta}\delta^{ij} + \rho u^i u^j\right) = -\frac{\partial}{\partial x^k}\left(\rho\bar{\theta}u^k\right)\delta^{ij} - \frac{2}{D}\rho\bar{\theta}\frac{\partial u^k}{\partial x^k}\delta^{ij} \\
&-\frac{\partial}{\partial x^k}(\rho u^i u^j u^k) - u^j \frac{\partial}{\partial x^i}\left(\rho\bar{\theta}\right) - u^i \frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\right),
\end{aligned}$$

is to be fed into Eq.(4.111) to allow for the substitution of the position and time cross derivative term:

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\rho\bar{\theta}\delta^{ij} + \rho u^i u^j\right) = -\frac{\partial}{\partial x^k}\left[\rho u^k\left(\bar{\theta}\delta^{ij} + u^i u^j\right)\right] \\
&-\frac{2}{D}\rho\bar{\theta}\frac{\partial u^k}{\partial x^k}\delta^{ij} - u^j \frac{\partial}{\partial x^i}\left(\rho\bar{\theta}\right) - u^i \frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\right). \qquad (4.132)
\end{aligned}$$

Finally we are able to write the addition of two terms proportional to τ in Eq. (4.113) in terms of the derivative of the viscosity stress tensor (Eq.(4.5)) by means of Eq.(4.132).

$$\begin{aligned}
& \frac{\partial}{\partial x^j}\frac{\partial}{\partial x^k}\left[\rho(u^k\delta^{ij}+u^j\delta^{ik}+u^i\delta^{jk})\bar{\theta}+\rho u^i u^j u^k\right]+\frac{\partial}{\partial x^j}\frac{\partial}{\partial t}\left[\rho\left(\bar{\theta}\delta^{ij}+u^i u^j\right)\right] \\
= & \frac{\partial}{\partial x^j}\frac{\partial}{\partial x^i}\left(\rho u^j\bar{\theta}\right)+\frac{\partial}{\partial x^j}\frac{\partial}{\partial x^j}\left(\rho\bar{\theta}u^i\right)-\frac{\partial}{\partial x^i}\left(\frac{2}{D}\rho\bar{\theta}\frac{\partial u^k}{\partial x^k}\right) \\
& -\frac{\partial}{\partial x^j}\left[u^j\frac{\partial}{\partial x^i}\left(\rho\bar{\theta}\right)\right]-\frac{\partial}{\partial x^j}\left[u^i\frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\right)\right] \\
= & \frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\frac{\partial u^j}{\partial x^i}\right)+\frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\frac{\partial u^i}{\partial x^j}\right)-\frac{\partial}{\partial x^i}\left(\frac{2}{D}\rho\bar{\theta}\frac{\partial u^k}{\partial x^k}\right) \\
= & \frac{\partial}{\partial x^j}\left[\rho\bar{\theta}\left(\frac{\partial u^j}{\partial x^i}+\frac{\partial u^i}{\partial x^j}-\frac{2}{D}\frac{\partial u^k}{\partial x^k}\delta^{ij}\right)\right]. \qquad (4.133)
\end{aligned}$$

Substituting this result in Eq.(4.113), we obtain the momentum conservation equation,

$$\frac{\partial}{\partial t}(\rho u^i)+\frac{\partial}{\partial x^j}\left[\rho\left(\bar{\theta}\delta^{ij}+u^i u^j\right)\right]-\frac{\partial\bar{\sigma}^{ij}}{\partial x^j}=0, \qquad (4.134)$$

also known as Quantum Navier-Stokes equation [42].

The energy conservation equation

Some identities are obtained here, similarly to the momentum equation case. From Eqs.(4.127) and (4.129), it follows that,

$$\begin{aligned}
& \frac{\partial}{\partial t}\left[(D+2)\rho\bar{\theta}u^j\right]=(D+2)u^j\frac{\partial}{\partial t}\left(\rho\bar{\theta}\right)+(D+2)\rho\bar{\theta}\frac{\partial u^j}{\partial t} \\
= & -(D+2)\left[\frac{\partial}{\partial x^k}\left(\rho\bar{\theta}u^j u^k\right)+\frac{2}{D}\rho\bar{\theta}\frac{\partial u^k}{\partial x^k}u^j+\bar{\theta}\frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\right)\right]. \qquad (4.135)
\end{aligned}$$

Using the continuity equation (Eq.(2.3)) and Eq.(4.127), one obtains that,

$$\begin{aligned}
& \frac{\partial}{\partial t}(\rho u^j\boldsymbol{u}^2)=\frac{\partial\rho}{\partial t}u^j\boldsymbol{u}^2+\rho\frac{\partial u^j}{\partial t}\boldsymbol{u}^2+2\rho u^j u^k\frac{\partial u^k}{\partial t} \\
= & -\frac{\partial}{\partial x^k}\left(\rho u^k u^j\boldsymbol{u}^2\right)-\frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\right)\boldsymbol{u}^2-2u^j u^k\frac{\partial}{\partial x^k}\left(\rho\bar{\theta}\right). \qquad (4.136)
\end{aligned}$$

Eqs.(4.135) and (4.136) allows to write the time dependent term of the position-time cross derivative in Eq. (4.124) as,

$$\begin{aligned}
& \frac{\partial}{\partial t}\left[\rho\boldsymbol{u}^2u^j+\rho\bar{\theta}(D+2)u^j\right]=-\frac{\partial}{\partial x^k}\left[\rho u^k u^j\boldsymbol{u}^2+(D+2)\rho\bar{\theta}u^j u^k\right] \\
& -\frac{2}{D}(D+2)\rho\bar{\theta}\frac{\partial u^k}{\partial x^k}u^j-\left[(D+2)\bar{\theta}+\boldsymbol{u}^2\right]\frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\right)-2u^j u^k\frac{\partial}{\partial x^k}\left(\rho\bar{\theta}\right). \qquad (4.137)
\end{aligned}$$

Next we deal with the terms proportional to τ in *the left side* of Eq.(4.124) and apply Eq.(4.137) to it. For this define,

$$\tau\left[\cdots\right] \equiv \frac{1}{2}\frac{\partial}{\partial x^j}\frac{\partial}{\partial x^k}\left[\rho \boldsymbol{u}^2 u^j u^k + \rho\bar{\theta}(D+4)u^j u^k + \rho\bar{\theta}\boldsymbol{u}^2\delta^{jk} + \rho\bar{\theta}^2(D+2)\delta^{jk}\right]$$
$$+\frac{1}{2}\frac{\partial}{\partial x^j}\frac{\partial}{\partial t}\left[\rho u^j \boldsymbol{u}^2 + \rho\bar{\theta}(D+2)u^j\right], \tag{4.138}$$

and substitute (4.137) into the above equation plus the cancelling of some terms, giving the final useful expression for the τ dependent terms of *the left side* of Eq.(4.124):

$$\tau\left[\cdots\right] = \frac{D+2}{2}\frac{\partial}{\partial x^j}\left(\rho\bar{\theta}\frac{\partial}{\partial x^j}\bar{\theta}\right) + \frac{\partial}{\partial x^j}\left[\rho\bar{\theta}u^k\left(\frac{\partial u^k}{\partial x^j} + \frac{\partial u^j}{\partial x^k} - \frac{2}{D}\frac{\partial u^l}{\partial x^l}\delta^{jk}\right)\right]. \tag{4.139}$$

The above expression is introduced into Eq.(4.124), added to the definitions of the dynamic viscosity (Eq.(4.6)), the viscosity stress tensor (Eq.(4.5)) and the thermal conductivity (Eq.(4.7)), which leads to

$$\frac{\partial}{\partial t}\left(\frac{\rho}{2}\boldsymbol{u}^2 + \frac{\rho}{2}D\bar{\theta}\right) + \frac{\partial}{\partial x^j}\left[\left(\frac{\rho}{2}\boldsymbol{u}^2 + \frac{\rho}{2}\bar{\theta}(D+2)\right)u^j + \tilde{Q}^j - u^k\bar{\sigma}^{j\,k}\right] = 0, \tag{4.140}$$

that is the *energy equation for quantum fluids* and the true heat flux vector, $\tilde{Q}^j$, is given by

$$\tilde{Q}^j = \bar{Q}^j - \frac{\partial}{\partial x^j}[\bar{\kappa}(g(z)-1)\bar{\theta}] \ , \ \bar{Q}^j \equiv -\bar{\kappa}\frac{\partial\bar{\theta}}{\partial x^j}. \tag{4.141}$$

4.3 Macroscopic equations from the BE and FD distribution functions

The conservation of mass is given by Eq.(4.104) and the momentum balance equation for quantum fluids is described by Eq.(4.134). Comparison between Eq.(2.25) and Eq.(4.134) shows that the classical and the quantum equations are the same provided that the true temperature θ is mapped into the pseudo temperature, $\bar{\theta}$. The same does not hold for the energy equations, namely, Eq.(2.29) and Eq.(4.140), as the dependence of the quantum case in the true temperature cannot collapse into the pseudo temperature. The fugacity z explicitly appears there through the function $g(z)$, Eq.(4.76). Thus the

writing of the energy equation solely in terms of pseudo variables is spoiled just by the extra term, that must be added to the pseudo heat flux vector, $\bar{Q}^j$, to obtain the true one, $\tilde{Q}^j$.

In conclusion it is remarkable that the replacement of $\tilde{Q}^j$ by $\bar{Q}^j$ in Eq.(4.140) renders the mass, momentum and energy equations for the quantum and classical fluids formally identical, provided that the density and the temperature are replaced by Eqs.(4.4) and (4.2), respectively. Another way to see this connection is by noticing that for the quantum problem all the explicit and *linear* dependence in the temperature appears through the pseudo temperature. This is the reason why the mass and momentum equations of quantum and classical cases are formally equivalent, but not the energy equation. The quantum energy equation has an extra *quadratic* dependence on the temperature brought by the function $g(z) - 1$, as already discussed. There is a link between this quadratic behaviour in the temperature and the $g(z)$ function, as shown by the identity below.

$$\theta^2 \frac{g_{\frac{D}{2}+2}(z)}{g_{\frac{D}{2}}(z)} = \bar{\theta}^2 g(z). \tag{4.142}$$

The quantum counterparts of the classical momentum and energy equations, namely, Eqs.(2.31) and (2.32), are given by

$$\rho \left(\frac{\partial}{\partial t} + u^j \frac{\partial}{\partial x^j} \right) u^i + \frac{\partial}{\partial x^j} \bar{P}^{i\,j} = 0, \tag{4.143}$$

and,

$$\frac{\partial}{\partial t} \left(\frac{D}{2} \rho \bar{\theta} \right) + \frac{\partial}{\partial x^j} \left(\frac{D}{2} \rho \bar{\theta} u^j \right) + \frac{1}{2} \left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i} \right) \bar{P}^{i\,j} + \frac{\partial}{\partial x^i} \tilde{Q}^i = 0, \tag{4.144}$$

respectively. We can define the pseudo stress tensor,

$$\bar{P}^{i\,j} \equiv \rho \bar{\theta} \delta^{i\,j} - \bar{\sigma}^{i\,j}. \tag{4.145}$$

We obtain the true thermal conductivity coefficient, κ_θ, and the chemical potential coefficient, κ_μ, through their definition:

$$\tilde{Q}^j = -\kappa_\theta \frac{\partial \theta}{\partial x^j} - \kappa_\mu \frac{\partial \mu}{\partial x^j}. \tag{4.146}$$

To derive the above coefficients, we write the pseudo heat flux vector as,

$$\tilde{Q}^j = \bar{\theta}\frac{\partial \bar{\kappa}}{\partial x^j} - \frac{\partial}{\partial x^j}\left[\bar{\kappa} g(z) \bar{\theta}\right]. \tag{4.147}$$

Firstly derive the function $g_\mu(z)$ of Eq.(4.3):

$$\frac{\partial g_\mu(z)}{\partial x^j} = g_{\mu-1}(z)\left(-\frac{\mu}{\theta}\frac{\partial \theta^2}{\partial x^j} + \frac{1}{\theta}\frac{\partial \mu}{\partial x^j}\right), \tag{4.148}$$

which leads to,

$$\frac{\partial \bar{\kappa}}{\partial x^j} = \rho\tau'\left\{\left[\left(\frac{D}{2}+1\right)\frac{g_{\frac{D}{2}+1}(z)}{g_{\frac{D}{2}}(z)} - \frac{\mu}{\theta}\right]\frac{\partial \theta}{\partial x^j} + \frac{\partial \mu}{\partial x^j}\right\}, \tag{4.149}$$

where $\tau' \equiv (D/2+1)\tau(1-\Delta t/2\tau)$. One also obtains that,

$$\frac{\partial\left(\bar{\kappa}\bar{\theta}g(z)\right)}{\partial x^j} = \rho\tau'\left\{\left[\left(\frac{D}{2}+2\right)\theta\frac{g_{\frac{D}{2}+2}(z)}{g_{\frac{D}{2}}(z)} - \mu\frac{g_{\frac{D}{2}+1}(z)}{g_{\frac{D}{2}}(z)}\right]\frac{\partial \theta}{\partial x^j} + \theta\frac{g_{\frac{D}{2}+1}(z)}{g_{\frac{D}{2}}(z)}\frac{\partial \mu}{\partial x^j}\right\} \tag{4.150}$$

The last two equations are introduced in Eq.(4.147) to obtain the coefficients κ_θ and κ_μ:

$$\kappa_\theta = \kappa\left[\left(\frac{D}{2}+2\right)\frac{g_{\frac{D}{2}+2}(z)}{g_{\frac{D}{2}}(z)} - \left(\frac{D}{2}+1\right)\left(\frac{g_{\frac{D}{2}+1}(z)}{g_{\frac{D}{2}}(z)}\right)^2\right] \tag{4.151}$$

$$\kappa_\mu = 0, \tag{4.152}$$

where κ is the MB (classical) thermal conductivity, given by Eq.(2.37). These are the coefficients obtained in Ref. [32] for the BGK-Boltzmann equation using the Uehling-Uhlenbeck approach.

4.4 The macroscopic equations for the non-expanded distribution function

In this section we show that the macroscopic equations obtained using the fourth order Hermite expansion ($\bar{f}^{(0)}$) and the non-expanded BE-FD distribution ($f^{(0)}$) give the same result.

For the continuity equation it's easy to see this because $\rho = \sum_\alpha \bar{f}^{(0)}_\alpha = \int f^{(0)} d^D\boldsymbol{\xi}$ and $\rho\boldsymbol{u} = \sum_\alpha \boldsymbol{\xi_\alpha}\bar{f}^{(0)}_\alpha = \int \boldsymbol{\xi} f^{(0)} d^D\boldsymbol{\xi}$. Notice the presence of the expanded function, $\bar{f}^{(0)}$, and the non-expanded one, $f^{(0)}$, in these expressions.

In the master equations for the conservation of momentum, Eq.(4.111), we see that the dependence of the distribution function is only on the tensors π^{ij} and π^{ijk}. So, if the tensors are made equal, the macroscopic equations will also be equal. Putting the BE-FD distribution function in the definition of π^{ij}, we have

$$\begin{aligned}\pi^{ij} &= \int \xi^i \xi^j f^{(0)} d^D\boldsymbol{\xi} \\ &= \frac{\delta^{ij}}{D}\int \frac{\eta^2 d^D\boldsymbol{\eta}}{z^{-1}e^{\frac{\eta^2}{2\theta}} \pm 1} + \rho u^i u^j \\ &= \frac{D\pi^{\frac{D}{2}}\delta^{ij}}{D\Gamma\left(\frac{D}{2}+1\right)}\int \frac{\eta^{D+1} d\eta}{z^{-1}e^{\frac{\eta^2}{2\theta}} \pm 1} + \rho u^i u^j,\end{aligned}$$

where we used the substitution $\boldsymbol{\eta} = \boldsymbol{\xi} - \boldsymbol{u}$. To obtain the BE-FD integral, we use another substitution, $x = \eta^2/2\theta$

$$\begin{aligned}\pi^{ij} &= \frac{\pi^{\frac{D}{2}}\delta^{ij}(2\theta)^{\frac{D}{2}+1}}{2\Gamma\left(\frac{D}{2}+1\right)}\int \frac{x^{\frac{D}{2}} dx}{z^{-1}e^x \pm x} + \rho u^i u^j \\ &= \rho(\bar{\theta}\delta^{ij} + u^i u^j). \qquad (4.153)\end{aligned}$$

From this equation we find the following identity

$$\int \eta^i \eta^j f^{(0)} d^D\boldsymbol{\eta} = \rho\delta^{ij}\bar{\theta}. \qquad (4.154)$$

Now, we calculate the tensor π^{ijk}

$$\pi^{ijk} = \int \xi^i \xi^j \xi^k f^{(0)} d^D\xi, \qquad (4.155)$$

using Eq.(4.154) and taking only the even terms,

$$\pi^{ijk} = \rho[\bar{\theta}(u^i\delta^{jk} + u^j\delta^{ik} + u^k\delta^{ij}) + u^i u^j u^k]. \qquad (4.156)$$

We conclude that Eqs.(4.153) and (4.156) are identical to Eqs.(4.112), and so, the same equation for conservation of momentum results from the full and the expanded approach.

Now, we use the same analysis for the master equation of energy, Eq.(4.120). We calculate the tensors ϕ, ϕ^j and ϕ^{jk}.

$$\begin{aligned}\phi &= \frac{1}{2}\int \boldsymbol{\xi}^2 f^{(0)} d^D\boldsymbol{\xi} \\ &= \rho\bar{\theta}\frac{D}{2} + \rho\boldsymbol{u}^2 \qquad (4.157)\end{aligned}$$

$$\begin{aligned}\phi^i &= \frac{1}{2}\int \boldsymbol{\xi}^2\xi^i f^{(0)} d^D\boldsymbol{\xi} \\ &= \frac{\rho}{2}u^i[\bar{\theta}(D+2)+\boldsymbol{u}^2] \end{aligned} \tag{4.158}$$

$$\begin{aligned}\phi^{jk} &= \frac{1}{2}\int \boldsymbol{\xi}^2\xi^j\xi^k f^{(0)} d\boldsymbol{\xi} \\ &= \frac{1}{2}\left(\int \eta^2\eta^j\eta^k f^{(0)} d^D\boldsymbol{\eta} + \rho u^j u^k D\bar{\theta} + 2\rho u^j u^k\delta^{jk}\bar{\theta}\right. \\ &\quad \left. +2\rho u^j u^k\delta^{jk}\bar{\theta} + \rho\boldsymbol{u}^2\delta^{jk}\bar{\theta} + \rho\boldsymbol{u}^2 u^j u^k\right) \end{aligned} \tag{4.159}$$

The first integral gives

$$\begin{aligned}&\int \frac{\boldsymbol{\eta}^2\eta^j\eta^k d^D\eta}{z^{-1}e^{\frac{\eta^2}{2\theta}}\pm 1} \\ =\ & \frac{\delta^{jk}}{D}\int \frac{\eta^4 d^D\boldsymbol{\eta}}{z^{-1}e^{\frac{\eta^2}{2\theta}}\pm 1} \\ =\ & \frac{\delta^{jk}\pi^{\frac{D}{2}}(2\theta)^{\frac{D}{2}+2}}{2\Gamma\left(\frac{D}{2}+1\right)}\int \frac{x^{\frac{D}{2}+1}dx}{z^{-1}e^x\pm 1} \\ =\ & \rho(D+2)\delta^{jk}\bar{\theta}^2 g(z) \end{aligned} \tag{4.160}$$

and using Eq.(4.154) we find

$$\begin{aligned}\phi^{jk} &= \frac{1}{2}\left[\rho(D+2)\delta^{jk}\bar{\theta}^2 g(z) + \rho\bar{\theta}\left(Du^j u^k + 4u^j u^k + \boldsymbol{u}^2\delta^{jk}\right) + \rho\boldsymbol{u}^2 u^j u^k\right] \\ &= \frac{\rho}{2}\left[(D+2)\delta^{jk}\bar{\theta}^2 g(z) + \bar{\theta}(D+4)u^j u^k + \bar{\theta}\boldsymbol{u}^2\delta^{jk} + \boldsymbol{u}^2 u^j u^k\right]. \end{aligned} \tag{4.161}$$

Again we find that full and the expanded distribution give the same result (see Eqs.(4.121), (4.122) and (4.123)). It means that the macroscopic equations found using the fourth order expansion and the non-expanded distribution function are exactly the same ones! Notice we made others approximations in our calculations to find macroscopic equations (e.g the Chapman Enskog expansion), but the truncation of the expansion of the distribution function causes no harm as it gives the correct answer. It shows the importance of the fourth order Hermite polynomial expansion to thermal LBM, even for the classical case.

4.5 The Hermite polynomial expansion to order N=3

This section provides a no-go theorem for the use of an Hermite polynomial expansion with terms lower than $N = 4$ in case of thermal fluids. Notice that the quantum fluid is necessarily thermal, but our considerations are valid for the classical thermal fluid too. The BE-FD equilibrium distribution function must be carried until $N = 4$ order to obtain meaningful results. We show that the $N = 3$ order simply does not correctly describe the energy equation. The BE-FD function equilibrium distribution function expanded until order $N = 3$ is given by,

$$\hat{f}_\alpha^{(0)} = w_\alpha \rho \Bigg\{ 1 - \frac{1}{2}\boldsymbol{u}^2 + (\boldsymbol{\xi}_\alpha \cdot \boldsymbol{u}) \left(1 - \frac{1}{2}\boldsymbol{u}^2 \right) + \frac{1}{2}(\boldsymbol{\xi}_\alpha \cdot \boldsymbol{u})^2 + \frac{1}{6}(\boldsymbol{\xi}_\alpha \cdot \boldsymbol{u})^3 \quad (4.162)$$
$$+ \left(\bar{\theta} - 1\right) \cdot \left[\frac{1}{2}(\boldsymbol{\xi}_\alpha^2 - D) + \frac{1}{2}(\boldsymbol{\xi}_\alpha \cdot \boldsymbol{u})(\boldsymbol{\xi}_\alpha^2 - D - 2) \right] \Bigg\}.$$

Notice that for the above equilibrium distribution function the fugacity z is only present through the pseudo temperature $\bar{\theta}$ of Eq.(4.2), but this is not so for the equilibrium distribution function of Eq.(4.75). This shows that the quantum and the classical macroscopic hydrodynamical equations are identical until $N = 3$ order by mapping the pseudo variables into their counterparts. In order $N = 4$ this mapping holds for the mass and momentum but not for the energy equation. This conclusion can be reached by analysing the $N = 3$ order construction of the momentum and energy tensors, given by Eqs.(4.112), (4.121), (4.122) and (4.123). Interestingly, the momentum tensors of Eq.(4.112) are the same in order $N = 3$ and $N = 4$, as seen below.

$$\sum_\alpha \xi_\alpha^i \hat{f}_\alpha^{(0)} = \rho u^i, \quad (4.163)$$

$$\sum_\alpha \xi_\alpha^i \xi_\alpha^j \hat{f}_\alpha^{(0)} = \rho \left(\bar{\theta}\delta^{ij} + u^i u^j \right), \quad (4.164)$$

$$\sum_\alpha \xi_\alpha^i \xi_\alpha^j \xi_\alpha^k \hat{f}_\alpha^{(0)} = \rho \left[\bar{\theta} \left(u^k \delta^{ij} + u^j \delta^{ik} + u^i \delta^{jk} \right) + u^i u^j u^k \right]. \quad (4.165)$$

Thus we conclude that to obtain Eq.(4.111) and Eq.(4.113) it is just enough to carry the expansion to order $N = 3$. Consequently the quantum Navier Stokes equation, namely, Eq.(4.134), is obtained in order $N = 3$ and higher order terms, such as $N = 4$ terms, do not contribute to it. Thus concerning the momentum equation, classical and quantum fluids have formally the same macroscopic description. However the same does not hold for the energy equation, as we learn by the expressions of the energy tensors in $N = 3$ order. They are given by,

$$\frac{1}{2}\sum_{\alpha}\boldsymbol{\xi_{\alpha}}^{2}\hat{f}_{\alpha}^{(0)} = \frac{1}{2}\rho\boldsymbol{u}^{2} + \frac{D}{2}\rho\bar{\theta}, \tag{4.166}$$

$$\frac{1}{2}\sum_{\alpha}\boldsymbol{\xi_{\alpha}}^{2}\xi_{\alpha}^{j}\hat{f}_{\alpha}^{(0)} = \frac{\rho}{2}\left[u^{j}\boldsymbol{u}^{2} + \bar{\theta}\left(D+2\right)u^{j}\right], \tag{4.167}$$

$$\frac{1}{2}\sum_{\alpha}\boldsymbol{\xi_{\alpha}}^{2}\xi_{\alpha}^{j}\xi_{\alpha}^{k}\hat{f}_{\alpha}^{(0)} = \frac{\rho}{2}\left[\left(D+4\right)u^{j}u^{k} + \boldsymbol{u}^{2}\delta^{jk} + \left(2\bar{\theta}-1\right)\left(D+2\right)\delta^{jk}\right]. \tag{4.168}$$

The last tensor, $\sum_{\alpha}\boldsymbol{\xi_{\alpha}}^{2}\xi_{\alpha}^{j}\xi_{\alpha}^{k}\hat{f}_{\alpha}^{(0)}/2$, differs from its $N = 4$ counterpart, as seen by comparison to Eq.(4.123). The first two other tensors are identical in $N = 3$ and $N = 4$ order, as seen by comparison to Eqs.(4.121) and (4.122). Thus with the exception of a single energy tensor all other ones are identical in $N = 3$ and $N = 4$ order. Nevertheless this single tensor renders the $N = 3$ energy equation unfit to describe the energy evolution of the quantum fluid. Hereafter we will develop a heuristic procedure to obtain the $N = 3$ tensor from its $N = 4$ counterpart, given by Eq.(4.123). Consider the following approximations in the $N = 4$ tensor, $\sum_{\alpha}\boldsymbol{\xi_{\alpha}}^{2}\xi_{\alpha}^{j}\xi_{\alpha}^{k}\hat{f}_{\alpha}^{(0)}/2 = \rho[\boldsymbol{u}^{2}u^{j}u^{k} + \bar{\theta}(D+4)u^{j}u^{k} + \bar{\theta}\boldsymbol{u}^{2}\delta^{jk} + \bar{\theta}^{2}g(z)(D+2)\delta^{jk}]$. Firstly drop the fourth power terms in the velocity. Notice that $\bar{\theta}-1$ is of the order of velocity square, as shown in section 3.2, and so, terms multiplied by the second power in the velocity are of maximum order, and therefore, also dropped. Apply $g(z) = 1$, as we know that such function does not exist in $N = 3$ order because it is not contained in $\hat{f}_{\alpha}^{(0)}$. Therefore take the above tensor in the limit that $\bar{\theta} = (\bar{\theta}-1)+1 \to 1$ and $\bar{\theta}^{2} = (\bar{\theta}-1)^{2} + 2\bar{\theta} - 1 \to 2\bar{\theta} - 1$ to obtain the above $N = 3$ expression for this tensor.

In conclusion, contributions of $N = 4$ order to the last tensor, $\sum_\alpha \boldsymbol{\xi_\alpha}^2 \xi_\alpha^j \xi_\alpha^k \hat{f}_\alpha^{(0)}/2$, are important and necessary to reach the energy equation of Eq.(4.124). Hence neither the energy of Eq.(4.140) nor the thermal coefficient of Eq.(4.151) can be obtained in $N = 3$ order.

Thus we have shown in this section that the $N = 3$ Hermite expansion yields an incorrect energy equation and therefore this order is not suitable to describe either the classical compressible thermal fluid or the quantum fluid. In conclusion the Hermite polynomial expansion must be carried to $N = 4$, in order to obtain meaningful results.

Chapter 5

Applications of the quantum hydrodynamics

In this chapter we apply the quantum hydrodynamic equations, i.e., Eqs.(4.104), (4.134) and (4.140), to a few situations..

5.1 Heat conduction in quantum fluid

In this section we derive the heat equation for quantum fluids.

Consider a quantum fluid with no macroscopic velocity $\boldsymbol{u}$ and a time independent density. The mass continuity equation,

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u^j)}{\partial x^j} = 0, \tag{5.1}$$

is naturally satisfied by the restrictions of the problem and it doesn't give any new information. The momentum equation, Eq.(4.134),

$$\rho \left(\frac{\partial}{\partial t} + u^j \frac{\partial}{\partial x^j} \right) u^i + \frac{\partial}{\partial x^j} \bar{P}^{ij} = 0, \tag{5.2}$$

has the the first term equal zero because it is multiplied by u^i, that is null. Since $\bar{P}^{ij} = \rho\bar{\theta}\delta^{ij} - \bar{\sigma}^{ij}$ and $\bar{\sigma}^{ij} = 0$ (see Eq.(4.5))

$$\frac{\partial}{\partial x^i}(\rho\bar{\theta}) = 0 \Rightarrow \rho\bar{\theta} = \text{constant in space.} \tag{5.3}$$

Using the above equation, we see that the second term in Eq.(4.144),

$$\frac{\partial}{\partial t}\left(\frac{D}{2}\rho\bar{\theta}\right) + \frac{\partial}{\partial x^j}\left(\frac{D}{2}\rho\bar{\theta}u^j\right) + \frac{1}{2}\left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i}\right)\bar{P}^{ij} + \frac{\partial \tilde{Q}^i}{\partial x^i} = 0, \tag{5.4}$$

is zero, and so is the third. Thus the energy equation becomes

$$\frac{D}{2}\rho\frac{\partial\bar{\theta}}{\partial t}+\frac{\partial}{\partial x^i}\left\{\bar{Q}^i-\frac{\partial}{\partial x^i}\left[\bar{\kappa}(g(z)-1)\bar{\theta}\right]\right\}=0.$$

Remembering that $\bar{Q}^i=-\bar{\kappa}\partial\bar{\theta}/\partial x^i$ and that $\bar{\kappa}$ is proportional to $\rho\bar{\theta}$, we find that $\bar{\kappa}$ can get outside the derivative

$$\frac{D}{2}\rho\frac{\partial\bar{\theta}}{\partial t}-\bar{\kappa}\frac{\partial}{\partial x^i}\left\{\frac{\partial\bar{\theta}}{\partial x^i}+\frac{\partial}{\partial x^i}\left[(g(z)-1)\bar{\theta}\right]\right\}=0.$$

Thus

$$\frac{D}{2}\rho\frac{\partial\bar{\theta}}{\partial t}-\bar{\kappa}\frac{\partial^2}{\partial x^i\partial x^i}\left[\bar{\theta}+(g(z)-1)\bar{\theta}\right]=0$$

and, finally

$$\frac{D}{2}\rho\frac{\partial\bar{\theta}}{\partial t}-\bar{\kappa}\frac{\partial^2}{\partial x^i\partial x^i}\left[g(z)\bar{\theta}\right]=0, \tag{5.5}$$

that is the *heat conduction equation for quantum fluids*. Defining the *thermal diffusivity* as $\alpha^2=\frac{2\bar{\kappa}}{D\rho}$, we have

$$\frac{\partial\bar{\theta}}{\partial t}-\alpha^2\frac{\partial^2}{\partial x^i\partial x^i}\left[g(z)\bar{\theta}\right]=0. \tag{5.6}$$

In classical case, $\bar{\theta}\to\theta$ and $g(z)\to 1$ in such a way that equation (5.6) becomes the already known classical heat conduction equation[1], $\partial\theta/\partial t=\alpha\nabla^2\theta$.

5.2 Quantum Bernoulli's equation

Consider a quantum incompressible ideal fluid, i.e., with no viscosity and with no circulation ($\nabla\times\boldsymbol{u}=0$) and in steady flow. In view of the vector identity

$$\boldsymbol{u}\times(\nabla\times\boldsymbol{u})=\frac{1}{2}\nabla(\boldsymbol{u}^2)-\boldsymbol{u}\cdot\nabla\boldsymbol{u}, \tag{5.7}$$

we can call Eq.(4.134) introducing an external conservative force per volume $\mathbf{f}$ on the right rand side

$$\rho\left(\frac{\partial}{\partial t}+u^j\frac{\partial}{\partial x^j}\right)u^i+\frac{\partial\bar{P}^{ij}}{\partial x^j}=f^i. \tag{5.8}$$

[1]See *http://mathworld.wolfram.com/HeatConductionEquation.html*

Substituting the term $\boldsymbol{u}\cdot\nabla\boldsymbol{u}$ of the identity (5.7) into (5.8),

$$\rho\frac{\partial u^i}{\partial t}+\frac{\rho}{2}\frac{\partial}{\partial x^i}(u^k u^k)-\rho[\boldsymbol{u}\times(\nabla\times\boldsymbol{u})]^i+\frac{\partial}{\partial x^j}\left[\bar{p}\delta^{ij}-\bar{\sigma}^{ij}\right]=f^i. \tag{5.9}$$

As there is no circulation, no viscosity and no velocity change with time,

$$\frac{\rho}{2}\frac{\partial}{\partial x^i}(u^k u^k)+\frac{\partial}{\partial x^j}[\bar{p}\delta^{ij}]=f^i. \tag{5.10}$$

Since the force is conservative, it may be written as a gradient of a potential $\mathbf{f}=-\rho\nabla\psi$, giving

$$\frac{\partial}{\partial x^i}\left[\frac{\boldsymbol{u}^2}{2}+\frac{\bar{p}}{\rho}+\psi\right]=0, \tag{5.11}$$

and we finally find the *Bernoulli's equation for quantum fluids*:

$$\frac{\boldsymbol{u}^2}{2}+\frac{\bar{p}}{\rho}+\psi=\text{constant}. \tag{5.12}$$

Let us analyze some limits of this equation. In the classical case, it's easy to see that Eq.(5.12) becomes the classical Bernoulli's equation [15], since the pressure is $\bar{p}=\rho\bar{\theta}$ and $\bar{\theta}\to\theta$. Considering, for example, the external force as the gravitational force, the potential energy will be $\psi=gz$, where g is the local gravitational acceleration and z is the height relative to some reference point.

Consider the situation where $\boldsymbol{u}$ and ψ are constants. Then the equation (5.12) gives that $\partial\bar{\theta}/\partial x^i=0$, which means that $\bar{\theta}$ is a constant. We apply this situation to another limit that of fermions near to the Fermi surface. This limit occurs when $\mu/\theta\gg 1$, where μ is the chemical potential. In this limit, the Fermi-Dirac integral $g_\nu(z)$ can be expanded as follows,

$$g_\nu(z)=\frac{(\mu/\theta)^\nu}{\Gamma(\nu+1)}\left[1+\nu(\nu-1)\frac{\pi^2}{6}\left(\frac{\theta}{\mu}\right)^2+\ldots\right]. \tag{5.13}$$

Thus, the pseudo-temperature expanded until second order of θ/μ is

$$\bar{\theta}=\theta\frac{g_{\frac{D}{2}+1}(z)}{g_{\frac{D}{2}}(z)}\approx\frac{\mu}{\frac{D}{2}+1}\left[1+\frac{D\pi^2}{6}\left(\frac{\theta}{\mu}\right)^2\right]. \tag{5.14}$$

In this case, the chemical potential and the temperature are related by the Eq.(5.14) or, arranging the terms, $\theta^2=a\mu-b\mu^2$, where a and b are constants. This is the equation of an ellipse.

5.3 Couette flow for quantum fluids

In the Couette flow there are two infinite parallel plates with a viscous fluid between them. The top plate is moving with velocity V and the bottom plate is at rest. Consider that the no-slip condition also holds for the quantum fluid[2], and the fluid moves with the top plate due to the viscous drag force and we have the profile shown in figure 5.1. We also admit that the plates are at different temperatures θ_a and θ_b. The Couette flow contains

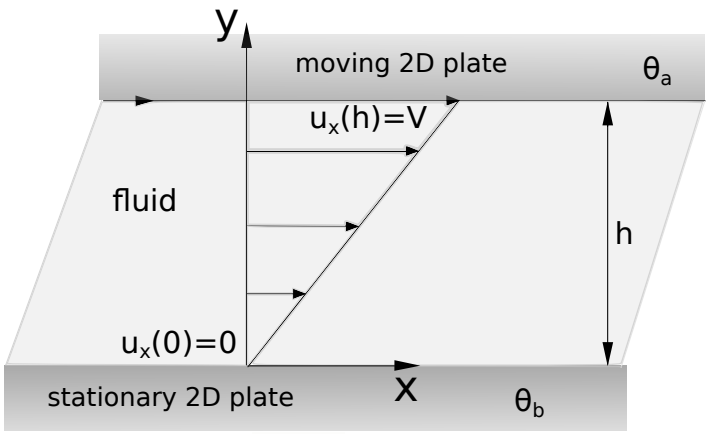

Figure 5.1: Scheme of Couette flow. Two parallel infinite plates separated by a distance h, where the top one moves with constant velocity V and the bottom plate is stationary. The temperature of two plates may be different.

two simplifying hypothesis. The first one is that the flow is steady, so that the velocity of fluid, and all others quantities, do not vary with time. The other assumption is that the velocity is parallel to the plates, and so, there is no pressure gradient perpendicular to plates. By the symmetry of the problem, the quantities can vary only in y direction. In this section we use the notation $x \equiv x_1$, $y \equiv x_2$, $u_x \equiv u_1$ and $u_y \equiv u_2$.

The continuity equation, Eq. (2.3), is trivially satisfied,

$$\underbrace{\frac{\partial \rho}{\partial t}}_{=0} + \frac{\partial(\rho u^i)}{\partial x^i} = 0 \Rightarrow \frac{\partial}{\partial x}(\rho u_x) + \frac{\partial}{\partial y}(\rho u_y) = 0,$$

[2]The no-slip condition states that the relative velocity between the solid boundary and the fluid layer that is in contact with the boundary is zero.

since the density has no dependence on time, $u_y = 0$ and the density and u_x are constants in x direction.

Recall that the momentum equation, Eq.(4.134), is

$$\underbrace{\frac{\partial}{\partial t}(\rho u^i)}_{=0} + \frac{\partial}{\partial x^j}\left[\rho(\bar{\theta}\delta^{ij} + u^i u^j)\right] - \frac{\partial \bar{\sigma}^{ij}}{\partial x^j} = 0,$$

where

$$\bar{\sigma}^{ij} = \bar{\eta}\left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i} - \frac{2}{D}\delta^{ij}\frac{\partial u^l}{\partial x^l}\right) \text{ and } \bar{\eta} = \rho\bar{\theta}\tau\left(1 - \frac{\Delta t}{2\tau}\right).$$

Using the hypothesis of our problem,

$$\frac{\partial u^l}{\partial x^l} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = 0,$$

so $\bar{\sigma}_{xx} = \bar{\sigma}_{yy} = 0$ and $\bar{\sigma}_{xy} = \bar{\sigma}_{yx} = \bar{\eta}\partial u_x/\partial y$. Thus, we have that

$$\frac{\partial \bar{\sigma}_{xy}}{\partial y} = 0 \Rightarrow \frac{\partial}{\partial y}\left(\bar{\eta}\frac{\partial u_x}{\partial y}\right) = 0, \text{ and} \tag{5.15}$$

$$\frac{\partial(\rho\bar{\theta})}{\partial y} = 0. \tag{5.16}$$

Next, we use the energy equation, Eq.(4.140)

$$\underbrace{\frac{\partial}{\partial t}\left(\frac{\rho}{2}\boldsymbol{u}^2 + \frac{\rho}{2}D\bar{\theta}\right)}_{=0} + \underbrace{\frac{\partial}{\partial x^j}\left[\left(\frac{\rho}{2}\boldsymbol{u}^2 + \frac{\rho}{2}\bar{\theta}(D+2)\right)u^j\right]}_{=0} + \frac{\partial}{\partial x^j}\left(\tilde{Q}^j - u^k\bar{\sigma}^{jk}\right) = 0 \tag{5.17}$$

with $\tilde{Q}^j$ being

$$\tilde{Q}^j = -\bar{\kappa}\frac{\partial\bar{\theta}}{\partial x^j} - \frac{\partial}{\partial x^j}\left[\bar{\theta}(g(z)-1)\bar{\theta}\right] \text{ and } \bar{\kappa} = \frac{D+2}{2}\rho\bar{\theta}\tau\left(1 - \frac{\Delta t}{2\tau}\right).$$

the first term in Eq.(5.17) is zero because there is no dependence on time and the second gives

$$\frac{\partial}{\partial x^j}\left[\left(\frac{\rho}{2}\boldsymbol{u}^2 + \frac{\rho}{2}\bar{\theta}(D+2)\right)u^j\right] = \underbrace{\frac{\partial}{\partial x}[(\ldots)u_x]}_{=0\,(\text{no x-dependence})} + \underbrace{\frac{\partial}{\partial y}[(\ldots)u_y]}_{=0\,(u_y=0)} = 0. \tag{5.18}$$

Calculating the remaining derivatives

$$\begin{aligned}\frac{\partial \tilde{Q}^j}{\partial x^j} &= \frac{\partial}{\partial x^j}\left\{-\bar{\kappa}\frac{\partial \bar{\theta}}{\partial x^j} - \frac{\partial}{\partial x^j}\left[\bar{\kappa}(g(z)-1)\bar{\theta}\right]\right\} \\ &= \frac{\partial}{\partial y}\left\{-\bar{\kappa}\frac{\partial \bar{\theta}}{\partial y} - \frac{\partial}{\partial y}\left[\bar{\kappa}(g(z)-1)\bar{\theta}\right]\right\} \end{aligned} \tag{5.19}$$

and

$$\frac{\partial}{\partial x^j}(u^k \bar{\sigma}^{jk}) = \frac{\partial}{\partial y}\left(\bar{\eta}\frac{\partial u_x}{\partial y}u_x\right) \tag{5.20}$$

since $\bar{\sigma}_{xx}u_x + \bar{\sigma}_{xy}u_y = 0$, $\bar{\sigma}_{xx}u_x = \bar{\sigma}_{xy}u_y = 0$ and $\bar{\sigma}_{yx}u_x = \bar{\eta}u_x \partial u_x/\partial y$. Therefore the energy equation becomes

$$\frac{\partial}{\partial y}\left\{\bar{\kappa}\frac{\partial \bar{\theta}}{\partial y} + \frac{\partial}{\partial y}[\bar{\kappa}(g(z)-1)\bar{\theta}]\right\} + \frac{\partial}{\partial y}\left(\bar{\eta}u_x\frac{\partial u_x}{\partial y}\right) = 0. \tag{5.21}$$

Using the definitions of $\bar{\eta}$ in Eq.(5.15)

$$\frac{\partial}{\partial y}\left[\rho\bar{\theta}\tau\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial u_x}{\partial y}\right] = \tau\left(1-\frac{\Delta t}{2\tau}\right)\underbrace{\frac{\partial}{\partial y}(\rho\bar{\theta})}_{=0\,\text{Eq.(5.16)}}\frac{\partial u_x}{\partial y} + \rho\bar{\theta}\tau\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial^2 u_x}{\partial y^2} = 0,$$

so

$$\frac{\partial^2 u_x}{\partial y^2} = 0. \tag{5.22}$$

This equation says that u_x is linear in y. Using the boundary condition that the velocity of top plate is V, Eq.(5.22) gives

$$u_x(y) = V\frac{y}{h}. \tag{5.23}$$

Indeed figure 5.1 shows a linear profile in the velocity. Now using the definitions of $\bar{\eta}$ and $\bar{\kappa}$ in Eq.(5.22)

$$\begin{aligned}\frac{D+2}{2}\left\{\rho\bar{\theta}\tau\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial^2\bar{\theta}}{\partial y^2} + \rho\bar{\theta}\tau\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial y}\left[(g(z)-1)\bar{\theta}\right]\right\} \\ +\rho\bar{\theta}\tau\left(1-\frac{\Delta t}{2\tau}\right)\frac{\partial}{\partial y}\left(u_x\frac{\partial u_x}{\partial y}\right) = 0 \quad .\end{aligned}$$

Finally,

$$\frac{D+2}{2}\left\{\frac{\partial^2\bar{\theta}}{\partial y^2}+\frac{\partial}{\partial y}[\bar{\theta}(g(z)-1)]\right\}+\left(\frac{\partial u_x}{\partial y}\right)^2=0, \tag{5.24}$$

where we used Eq.(5.22) to find $\frac{\partial}{\partial y}\left(u_x\frac{\partial u_x}{\partial y}\right)=\left(\frac{\partial u_x}{\partial y}\right)^2$. This equation can be written as

$$\frac{D+2}{2}\left\{\frac{\partial^2\bar{\theta}}{\partial y^2}+\frac{\partial}{\partial y}[\bar{\theta}(g(z)-1)]\right\}+\left(\frac{V}{h}\right)^2=0, \tag{5.25}$$

This is the differential equation that gives the temperature behavior of the temperature in Couette flow for quantum fluids. This equation can't be solved analytically for general case, so we restrict our treatment to classical one.

In classical limit, the function $g(z)\to 1$ and $\bar{\theta}\to\theta$. Thus, the Eq.(5.25) becomes [8]

$$\frac{D+2}{2}\frac{\partial^2\theta}{\partial y^2}=-\left(\frac{V}{h}\right)^2, \tag{5.26}$$

that has the following solution

$$\theta(y)=\left(\frac{V}{h}\right)^2\frac{2}{D+2}\frac{y(h-y)}{2}+\theta_a\frac{y}{h}+\theta_b\left(1-\frac{y}{h}\right), \tag{5.27}$$

where we used the boundary condition for temperature (see figure 5.1).

So, in this chapter, we saw three examples of applications of the conservations equations for quantum fluids, which gives some intuition about them.

Chapter 6

Numerical results

In this chapter we implement the quantum LBM developed in the previous chapters as a computer program. We used the dilute fluid approximation, because it is simpler implement and to stablish the initial conditions, but it was important as a first application of quantum LBM. We could study the energy conservation and temperature behaviour for two different initial conditions.

6.1 The dilute quantum fluid

We develop here the approximation of the dilute quantum (BE-FD) system, which is very near to the classical (MB) limit. This is the limit of small fugacity, $z \ll 1$ taken in the function of Eq.(4.3) [23]:

$$g_\nu(z) = z \mp \frac{z^2}{2^\nu} + \cdots \tag{6.1}$$

where the assignment is (+) BE and (-) FD, respectively. We intend to carry here just the first order corrections to the classical (MB) fluid which are linear in the fugacity. Then we Taylor expand the function $g(z)$ to obtain that,

$$g(z) = 1 \mp \frac{z}{2^{\frac{D}{2}+2}} + \cdots \tag{6.2}$$

In this order the density and the pseudo temperature are given by,

$$\rho = (2\pi\theta)^{\frac{D}{2}}\, z + \cdots \tag{6.3}$$

$$\bar{\theta} = \theta\left(1 \pm \frac{z}{2^{\frac{D}{2}+2}} + \cdots\right). \tag{6.4}$$

Within this order we can write the fugacity and so the function $g(z)$ in terms of the density and of the pseudo temperature,

$$g \approx 1 \mp \frac{1}{2^{\frac{D}{2}+2}} \frac{\rho}{\left(2\pi\bar{\theta}\right)^{\frac{D}{2}}} \tag{6.5}$$

under the assumption that

$$z \approx \frac{\rho}{\left(2\pi\bar{\theta}\right)^{\frac{D}{2}}} \ll 1. \tag{6.6}$$

Under this approximation the function g can be brought back to the BE-FD equilibrium distribution function of Eq.(4.77) that becomes a function of ρ, $\bar{\theta}$ and $\boldsymbol{u}$.

$$\begin{aligned} f_\alpha^{(0)} = w_\alpha \rho \Bigg\{ & 1 + (\boldsymbol{\xi}_\alpha \cdot \boldsymbol{u})\left(1 - \frac{1}{2}\boldsymbol{u}^2\right) + \frac{1}{6}(\boldsymbol{\xi}_\alpha \cdot \boldsymbol{u})^3 + (\boldsymbol{\xi}_\alpha \cdot \boldsymbol{u})^2\left(\frac{1}{2} - \frac{1}{4}\boldsymbol{u}^2\right) \\ & - \frac{1}{2}\boldsymbol{u}^2 + \frac{1}{8}\boldsymbol{u}^4 + \frac{1}{24}(\boldsymbol{\xi}_\alpha \cdot \boldsymbol{u})^4 + \left(\bar{\theta} - 1\right) \cdot \Bigg[\frac{1}{2}(\boldsymbol{\xi}_\alpha^2 - D) + \frac{1}{2}(\boldsymbol{\xi}_\alpha \cdot \boldsymbol{u})(\boldsymbol{\xi}_\alpha^2 - D - 2) \\ & + \frac{1}{4}(\boldsymbol{\xi}_\alpha \cdot \boldsymbol{u})^2(\boldsymbol{\xi}_\alpha^2 - D - 4) + \frac{1}{4}\boldsymbol{u}^2(D + 2 - \boldsymbol{\xi}_\alpha^2)\Bigg] + \frac{1}{8}\Bigg[\bar{\theta}^2\left(1 \mp \frac{1}{2^{\frac{D}{2}+2}} \frac{\rho}{\left(2\pi\bar{\theta}\right)^{\frac{D}{2}}}\right) \\ & - 2\bar{\theta} + 1\Bigg] \cdot [\boldsymbol{\xi}_\alpha^4 + (D+2)(D - 2\boldsymbol{\xi}_\alpha^2)]\Bigg\}. \end{aligned} \tag{6.7}$$

Thus the LBM for the dilute quantum fluid can be developed through the variables density ρ, macroscopic velocity $\boldsymbol{u}$ and pseudo temperature $\bar{\theta}$. The latter is related to the true temperature θ through the relation,

$$\overline{\theta} \cong \theta \pm \frac{\rho}{16\pi}, \tag{6.8}$$

where the $+$ and $-$ signs applies to fermions and bosons, respectively.

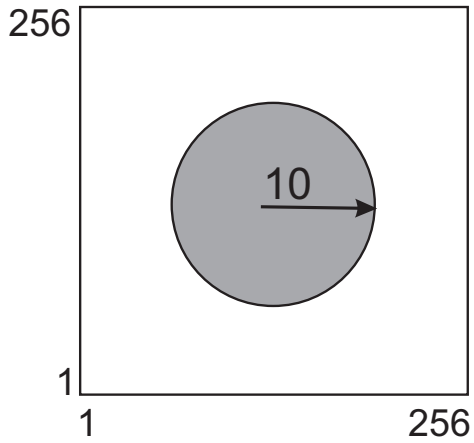

Figure 6.1: Pictorial view of the initial condition taken in a two-dimensional cell of 256^2 points with periodic boundary conditions. The outward velocity (or the density) takes distinct values inside and outside the circle of radius 10, while the remaining variables are taken homogeneous throughout the cell.

6.2 Numerical results

In this section we use the LBM based on the present $N = 4$ order theory to numerically solve the dilute quantum fluid. We find that the energy is indeed conserved in $D = 2$ under periodic boundary conditions and some initial conditions that trigger a time evolution where motion and heat occur simultaneously [7]. The initial conditions are associated to a circle of radius R located at the center of the cell, where one of the variables, among the temperature θ, velocity $\boldsymbol{u}$, and the density ρ, assumes a special value, whereas the other two are taken constant throughout the cell. A pictorial view of such initial conditions is shown in Fig. 6.1. We work with a grid of $A_{cell} = 256^2$ points, and in these units $R = 10$. We take for the time step of Eq.(3.72) $\tau/\Delta t = 0.58$. We use in this section the concept of a real temperature T connected to the reduced one by $T \equiv c_s^2\theta$, where c_s is a distinct numerical parameter for each of the lattices D2V17 and D2V37 (see figure 6.2), This parameter makes equal to one the smallest non-zero microscopic velocity along the axis [33]. In dimensionless units c_s plays the role of the speed c_r, defined by Eq.(3.30). The time evolution of the system is a multiple of the computer steps performed in our numerical procedure. Since our goal is to verify that the total energy remains constant

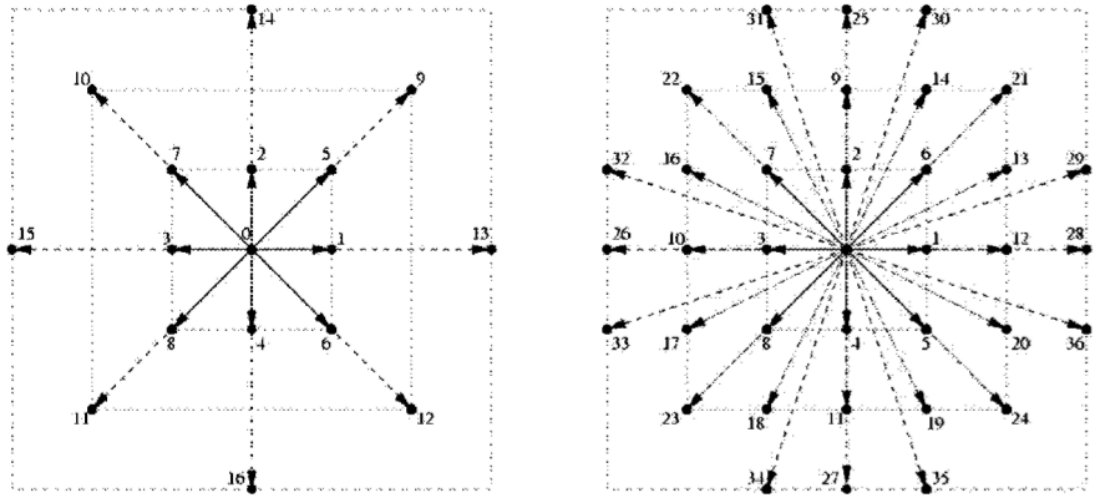

Figure 6.2: The figure on the left shows the D2Q17 lattice and, on the right, we see the D2V37 lattice. Taken from Ref. [34]

in the cell at any time step, we define the following sums over all cell points, which are the average values of the kinetic and the thermal energies in the cell.

$$E_{kin} \equiv \frac{1}{A_{cell}} \sum_{cell} \frac{1}{2} \rho \boldsymbol{u}^2 \tag{6.9}$$

$$E_{therm} \equiv \frac{1}{A_{cell}} \sum_{cell} \frac{D}{2} \rho \bar{\theta}, \text{ and} \tag{6.10}$$

$$E_{total} \equiv E_{kin} + E_{therm}, \tag{6.11}$$

In our numerical study we assume identical initial conditions for the BE, FD and MB cases, which means that they start with the same density, temperature and velocity. Thus the initial kinetic energy of Eq.(6.9) is the same for the three cases, but not the thermal energy of Eq.(6.10) since the initial pseudo temperature is not the same for the three cases, according to Eq.(6.8), being greater for fermions and smaller for bosons, as compared to the classical case.

To perform numerical calculations we must employ a concrete realization of the weights and microscopic velocities that satisfy the algebra of Eqs.(3.52) to (3.58). This assures that the Gauss-Hermite quadrature is being correctly performed. We choose the so-called D2V17 [31] and D2V37 [33] microscopic velocity lattices. It is important to make

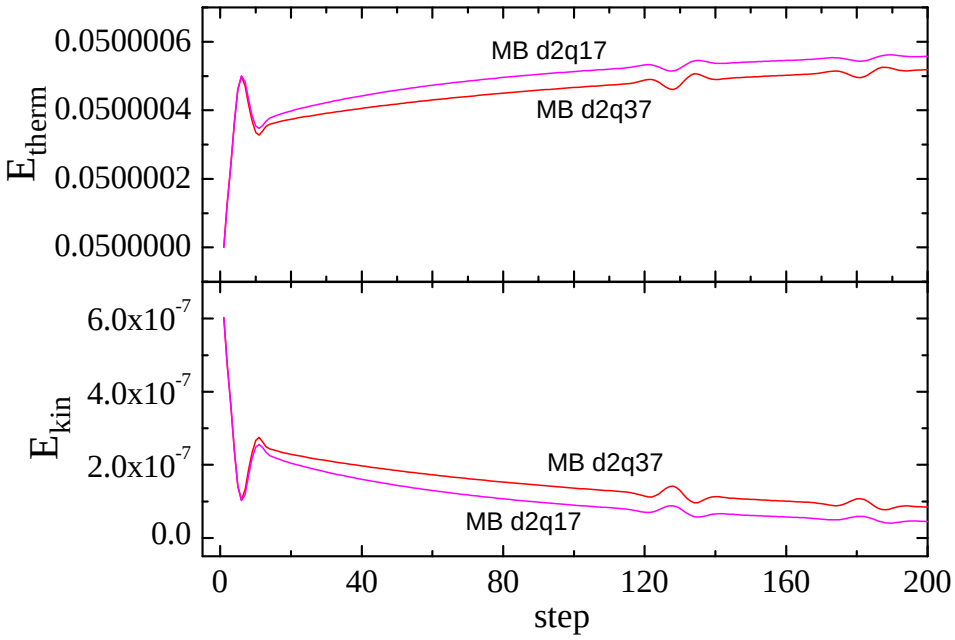

Figure 6.3: The thermal and the kinetic energies for the Maxwell-Boltzmann distribution, with the circle of radial velocity as initial condition, are shown here for the first 200 time steps, using both the D2V17 and D2V37 lattices. For time step 118 the travelling front wave hits the side of the unit cell.

a few considerations about these lattices regarding their ability to give the expected answers. This ability relies on the order of the maximum power of the microscopic velocity polynomial contained in the equilibrium distribution function and also the calculated moments. The equilibrium distribution function has maximum order $f_\alpha^{(0)} \sim \xi_\alpha^N$, for $N = 3$ and $N = 4$, as seen from Eq.(4.162) and Eq.(4.77), respectively. For computer purposes the highest moment that must be calculated is the energy, which is of order ξ_α^2. Thus the chosen microscopic velocity lattice must correctly account for the sums of the kind Eqs.(3.52) to (3.58), which means ξ_α^5 for $N = 3$ and ξ_α^6 for $N = 4$. According to Ref. [31] these calculations can be correctly done in the d2q9 and D2V17 algebras for $N = 3$ and $N = 4$, respectively. Thus we conclude that D2V17 and D2V37 can be used for the numerical treatment of the present $N = 4$ order LBM. Nevertheless to apply the Chapman-Enskog analysis and derive the equation for energy, one must compute the

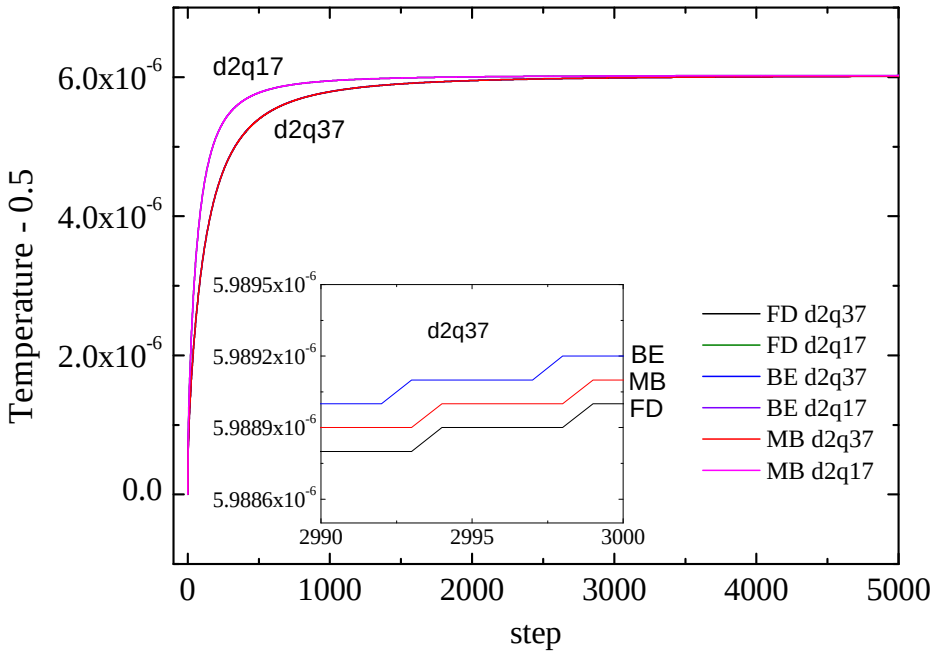

Figure 6.4: The deviation of the temperature from its initial value is shown here for the first 5000 time steps using the circle of velocity as initial condition. The the splitting among the FD, MB and BE distribution curves is very small in comparison to the D2V17 and D2V37 lattice splitting and for this reason not observable. The inset shows for a particular time step window the splitting of the temperature deviation among the three distributions for the D2V37 lattice.

moment $\phi^{jk} \sim \xi_\alpha^4 f_\alpha^{(0)}$. Hence in this case the microscopic velocity lattice must correctly account for sums beyond Eqs.(3.52) to (3.58), which means of the order ξ_α^7 for $N = 3$ and ξ_α^8 for $N = 4$. Thus for this purpose the D2V17 lattice is limited to $N = 3$ [31] and cannot be used $N = 4$. For such purpose $N = 4$ demands a higher order lattice, such as D2V37 [33].

6.2.1 Velocity initial conditions

Under this initial condition $\boldsymbol{u}$ is non-zero inside a circle of radius R, where the outward component is equal to 0.02 in reduced units, being zero outside the circle. Thus at the beginning radial motion is set for a dilute quantum fluid of constant density, $\rho = 0.1$, and temperature, $T = 0.5$, in the unit cell. This initial motion immediately generates

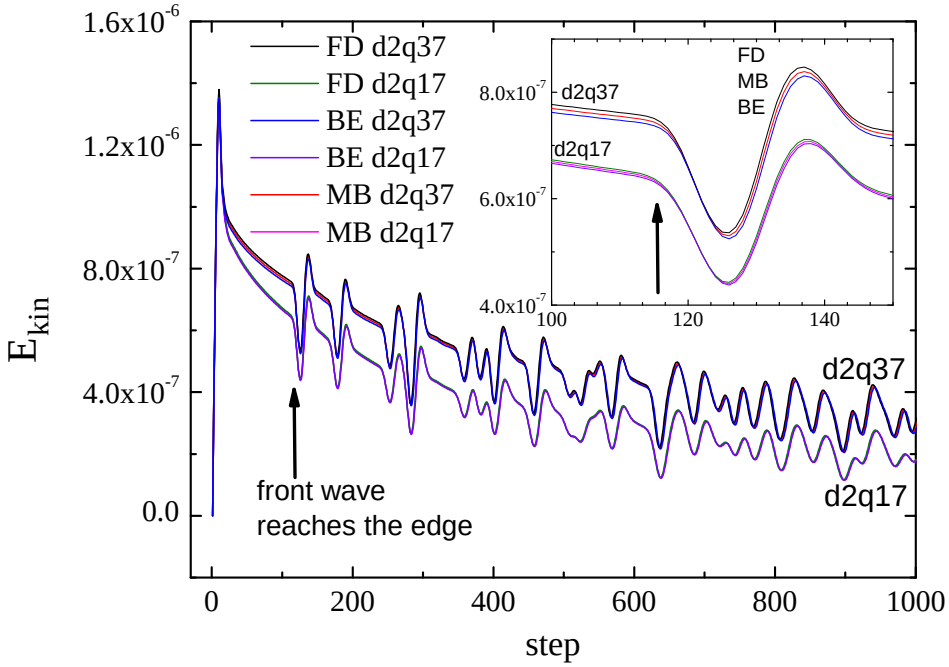

Figure 6.5: The Kinetic energy of the FD, MB and BE distributions using the D2V17 and D2V37 lattices is shown here for the first 1000 time steps. The initial condition used is of the circle of density. The inset shows in a particular time step window the splitting of the kinetic energy among the three distributions for both D2V17 and D2V37 lattices.

friction and subsequent heating that raises the temperature. Fig. 6.3 shows the time step evolution of E_{kin} and E_{therm} and the most important aspect found in these two plots is that their sum is a constant which is E_{total}, as given by Eq.(6.11). E_{kin} follows the trend of decrease in time, and eventually must vanish, while E_{therm} increases and tends to stabilize, though such behaviours are just suggested in the first 200 steps of Fig. 6.3. This figure only intends to display the evolution immediately after the initial condition. To reach a nearly steady state of zero velocity and stable temperature simulations up to 20.000 steps must be carried. The two employed lattices, namely D2V17 and D2V37, give the same qualitative results for the time evolution of the system, but their numerical difference hinders the splitting among the BE, FD and MB curves for each lattice as they fall very close to each other. Notice the non-zero initial value of E_{kin}, due to the initial velocity condition. After a few steps E_{kin} drops to a local minimum, which is a

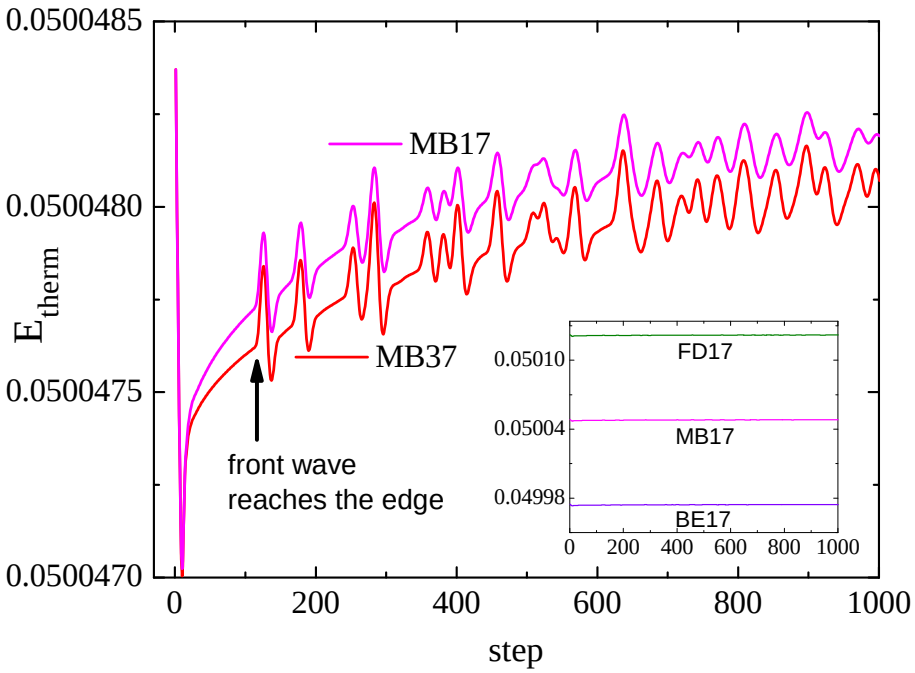

Figure 6.6: The thermal energy of the MB distribution using the D2V17 and D2V37 lattices is shown here for the first 1000 time steps. The initial condition used is that of the circle of density. The inset shows in a particular time step window the splitting of the kinetic energy among the three distributions for the D2V17 lattice.

local maximum for E_{therm}, meaning that friction caused by motion raises the temperature but in such a way that E_{total} is conserved. After 118 steps the front wave raised by the initial condition reaches the side of the unit cell. Notice that this number coincides with the number of grid points between the circle and the unit cell side, namely, (256-20)/2. In the numerical algorithm the speed of propagation is one, thus the number of steps required for the signal reach the border is the number of grid points itself. Indeed Fig. 6.3 shows a hilly behaviour starting nearly at 120 steps, a consequence of the interference of incoming waves from the neighbour cells. Fig. 6.4 shows the evolution of the temperature deviation from its initial value of $T = 0.5$. After 5000 steps the D2V17 and the D2V37 converge basically to the same final temperature which is just 6.0 10^{-6} above the initial one. Interestingly there is also oscillatory behaviour in the deviated temperature though much less perceptible than in Fig. 6.3. The inset of Fig. 6.4 shows the splitting between

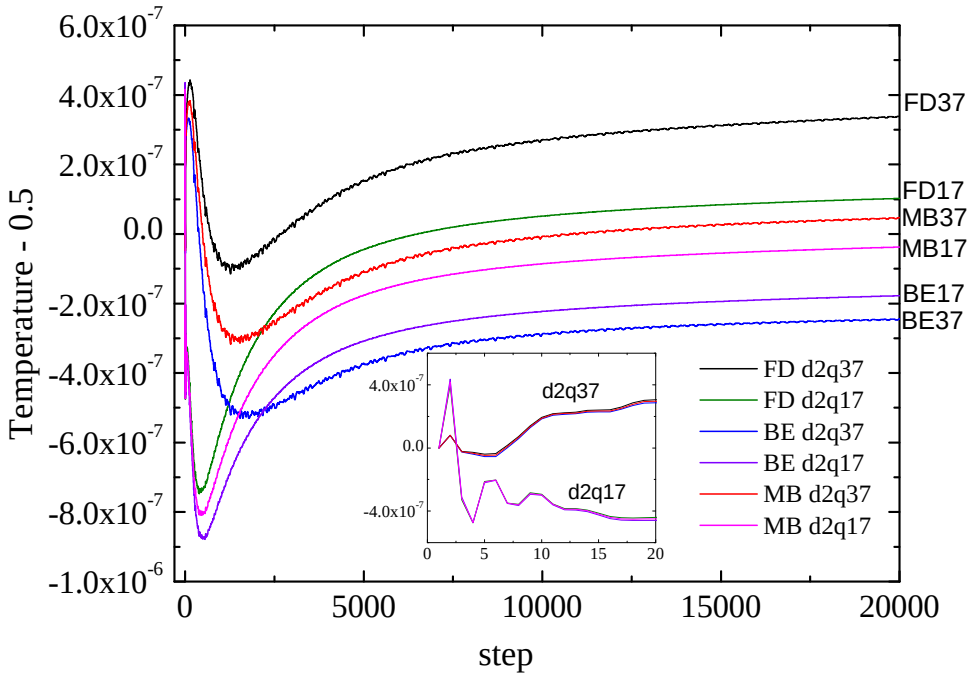

Figure 6.7: The temperature deviation from its initial value is shown here for the case of a circle of density as initial condition for the first 20000 time steps. The curves for the three distributions and the two lattices are clearly seen here. The inset shows the first 20 time steps.

the BE, FD and MB cases in a particular time step window. Indeed one observes that this splitting between the three statistics is of order 10^{-9} whereas the differences between D2V17 and D2V37 is of order 10^{-6}.

6.2.2 Density initial conditions

Under this initial condition the density is $\rho = 0.12$ inside and $\rho = 0.1$ outside the circle of radius R. The initial temperature is $T = 0.5$ and the macroscopic velocity $\boldsymbol{u}$ is zero everywhere. Though there is no initial motion, the non homogeneous density distribution sets a pressure front. The higher density at the center means higher pressure that forces motion outward the circle, and so, generates friction, heating and raise of the temperature in the cell. The first 1000 steps of E_{kin} are shown in Fig. 6.3. Notice that it starts from zero and the oscillatory behavior set by the entrance of wave fronts from neighbor cells

is well described by the D2V17 and D2V37 lattices since their numerical differences are in the range of 10^{-7}. In this case too the difference among the three distributions is hidden by the lattice difference, shown in the inset for a chosen window of time steps for both lattices. The trend towards kinetic energy decay is seen in this figure though the convergence towards a steady state is only suggested by this figure. To really see it a larger window must be taken. The time step evolution of E_{therm} is shown in Fig.(6.6). E_{therm} experiments a sudden drop to allow for the increase of E_{kin} (Fig.(6.5)) as the system starts motion due to pressure unbalance. As in the previously case, E_{total} is absolutely conserved to machine precision, in our case tested to order 10^{-10}. The inset of this plot shows the splitting of the three distributions within the first 1000 steps. Notice that such values are distinct because we chose the same initial θ for the three distributions, which means different $\bar{\theta}$ in the three cases. Finally we address the evolution of the temperature deviation from its initial value $T = 0.5$ in Fig.(6.7) within the full time step window studied, namely 20000 steps. The very first 20 steps, shown in the inset, indicate that the initial temperature is the same in all cases. However the final ones are different. The D2V17 reaches a final temperature deviation at a value slightly lower that the D2V37 case by an order of magnitude of 10^{-7}. The final deviation is higher for the FD distribution and lower for the BE. We notice during evolution a drop to a minimum of temperature required to accommodate the kinetic expansion caused by the pressure unbalance in an energy conserving scenario.

Chapter 7

Conclusion

In this thesis we have applied the fourth order Hermite polynomial expansion procedure, previously used for the classical compressible thermal fluid, to the quantum fluid. In this way we obtained the macroscopic hydrodynamical equations of the quantum fluid from a Chapman-Enskog analysis of the BGK-Boltzmann equation. The classical fluid is described by the Maxwell-Boltzmann equilibrium distribution function whereas the quantum ones by the Bose-Eisntein and Fermi-Dirac equilibrium distribution functions for bosons and fermions, respectively. We conclude that the construction of an LBM for the quantum fluid, similarly to the case of the thermal compressible classical fluid, requires the Hermite polynomial expansion to be carried until the fourth order in order to obtain the correct energy equation, which besides the mass and momentum equations, is also needed for a full description of friction-heating processes. We show that the viscosity and thermal coefficients, namely η and κ, of the BGK-Boltzmann quantum fluid, previously obtained through the Uehling-Uhlenbeck approach [32, 42], can only be retrieved in the fourth order, and not in lowest order. Therefore halting the Hermite polynomial expansion to third order, as done in Ref. [42], impairs the derivation of the correct energy equation of the quantum fluid. Similarly the macroscopic hydrodynamical equations obtained by Yang et al., Ref. [12], do not correctly describe the energy balance equation because they are limited to the third order. Although Ref. [42] provides the general form of the macroscopic hydrodynamical equations for the BGK-Boltzmann quantum fluid, it does

not express these equations in terms of the local macroscopic fields, namely, the chemical potential $\mu(\boldsymbol{x})$ (or the fugacity $z(\boldsymbol{x})$), the local temperature $\theta(\boldsymbol{x})$, and the local velocity $\boldsymbol{u}(\boldsymbol{x})$. In this thesis we obtained the macroscopic hydrodynamical equation in terms of the above macroscopic variables. We use the so-called d2V17 and d2V37 [33, 34] to treat the dilute limit of the quantum fluid where particles are so far a part that they behave almost like classical particles. We consider this example because it is the simples possible one. Nevertheless we stress that the present method is not limited to the dilute case and can be applied to other very interesting situations, such as the description of electrons in metals [13] and Bose-Eistein condensates [22]. We foresee much simplicity in the former case, as one can take the so-called Sommerfeld expansion [23, 27] and treat fermions near to the so-called Fermi surface. We expect that the present formulation will allow for the easy treatment of metals in presence of inhomogeneities, such as caused by local fields and non-metallic islands and also in arbitrary geometries. Finally we have considered in this thesis special limits of the quantum macroscopic hydrodynamical equations, such is the treatment of Couette's flow. We have derived a heat equation appropriate for the quantum fluid.

In more details we summarize blow the main achievements of this thesis. We obtained the equilibrium distribution function of the Bose-Einstein (BE) and Fermi-Dirac (FD) expanded until fourth order in Hermite polynomials, namely, Eq.(4.75), or equivalently, Eq.(4.77). We also obtained the Maxwell-Boltzmann (MB) equilibrium distribution function by Taylor expansion, namely, Eq.(3.37). In the classical limit the fourth BE-FD equilibrium distribution function becomes the Taylor expanded MB equilibrium distribution function. All our results are obtained in D dimensions, a feature that generalizes previous results discussed in the literature [32, 42]. Next we derived the macroscopic hydrodynamical equations for the BE-FD cases, Eq.(4.134) and Eq.(4.140), and showed that they become their MB counterparts, Eq.(2.25) and Eq.(2.29) in the classical limit, where BE, FD and MB statistics coincide. The viscosity and the thermal coefficients,

given by Eq.(4.6) and Eq.(4.151), respectively, are the ones previously derived in Ref. [32] by another method. We showed in Section 4.5 that the third order Hermite expansion yields an incorrect energy equation and therefore this order is not suitable to describe either the classical or the quantum fluid. The fourth order FD-BE fluid equations cannot be generally mapped into the MB ones for arbitrary fugacity. However this mapping, as found in this dissertation, is always possible at the third expansion level. This shows, once again, that the third order can not be correct. The fourth macroscopic hydrodynamical equations of the FD-BE fluids display an interesting property. To better understand this property we introduce the notation of *pseudo* variables, represented by a *bar* on the top of the corresponding variable. The property corresponds to the mapping of the *pseudo* variables into their counterparts, which leads the (BE-FD) quantum equations into the (MB) classical ones. However this mapping is not prefect, and is spoiled by a single term in the heat flow term of the energy equation, as seen in Eq.(4.141). We notice that Love and Boghosian [17] found that any equilibrium distribution that obeys isotropy and galilean invariance results in the same general form for the hydrodynamic equations [5]. Under such premises the BE and FD statistics have exactly one new extra term in the fluid equations as compared to the MB case, similar to the present findings.

Finally we explicitly constructed a LBM for the quantum fluids using the corresponding fourth order LBM scheme and obtain some numerical results in the limit of dilute quantum fluids. In this dilute limit the BE and FD are small corrections to the MB statistics. This is the limit where the average distance between particles is much larger than the thermal de Broglie wavelength. There is no overlap between the individual wave functions and the particles can not condense into a single quantum state. Our numerical analysis is based on some two-dimensional lattices [31,33], the so-called d2V17 and d2V37 lattices. Thus we are able to check that indeed quantum fluid motion generates friction and the heat created results into a temperature change such that the total energy remains conserved during a time evolution process. Our numerical study is restricted to an adia-

batic process as there is no external contact or force. We treat a two-dimensional system under periodic boundary conditions, thus without external borders and with no external applied force, just an initial displacement from equilibrium set by the initial conditions.

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2, 14, 59, 85, 86

Appendix A

Hermite polynomials

In this appendix, we introduce some important concepts related to Hermite polynomials that are used in this thesis.

The N^{th} order Hermite polynomial is defined by the Rodrigues' formula [14],

$$H^{i_1 i_2 \ldots i_N}(\boldsymbol{\xi}) = \frac{(-1)^N}{\omega(\boldsymbol{\xi})} \frac{\partial^N \omega(\boldsymbol{\xi})}{\partial \xi^{i_1} \partial \xi^{i_2} \ldots \partial \xi^{i_N}}, \tag{A.1}$$

where,

$$\omega(\boldsymbol{\xi}) \equiv \frac{1}{(2\pi)^{\frac{D}{2}}} \exp\left(-\frac{\boldsymbol{\xi}^2}{2}\right), \tag{A.2}$$

is the gaussian function. The orthonormality of the Hermite polynomials, $H^{i_1 i_2 \ldots i_N}(\boldsymbol{\xi})$, is given by,

$$\begin{aligned} &\int d^D \boldsymbol{\xi}\, \omega(\boldsymbol{\xi}) H^{i_1 i_2 \ldots i_N}(\boldsymbol{\xi}) H^{j_1 j_2 \ldots j_M}(\boldsymbol{\xi}) \\ &= \delta^{NM} (\delta^{i_1 j_1} \delta^{i_2 j_2} \ldots \delta^{i_N j_N} + \text{all permutations of j's}). \end{aligned} \tag{A.3}$$

The lowest order Hermite polynomials are easily derived from Eq.(A.1):

$$H(\boldsymbol{\xi}) = 1 \tag{A.4}$$

$$H^i(\boldsymbol{\xi}) = \xi^i \tag{A.5}$$

$$H^{ij}(\boldsymbol{\xi}) = \xi^i \xi^j - \delta^{ij} \tag{A.6}$$

$$H^{ijk}(\boldsymbol{\xi}) = \xi^i\xi^j\xi^k - (\xi^i\delta^{jk} + \xi^j\delta^{ik} + \xi^k\delta^{ij}) \tag{A.7}$$

$$\begin{aligned} H^{ijkl}(\boldsymbol{\xi}) &= \xi^i\xi^j\xi^k\xi^l - (\xi^i\xi^j\delta^{kl} + \xi^i\xi^k\delta^{jl} + \xi^i\xi^l\delta^{jk} \\ &\quad +\xi^j\xi^k\delta^{il} + \xi^j\xi^l\delta^{ik} + \xi^k\xi^l\delta^{ij}) + \delta^{ijkl}. \end{aligned} \tag{A.8}$$

where the symbol $\delta^{\cdots}$ is described in section 3.3. The following integrals over the gaussian function of Eq.(A.2) are a consequence of the orthonormality of the Hermite polynomials:

$$\int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi}) = 1 \tag{A.9}$$

$$\int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi})\xi^i = 0 \tag{A.10}$$

$$\int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi})\xi^i\xi^j = \delta^{ij} \tag{A.11}$$

$$\int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi})\xi^i\xi^j\xi^k = 0 \tag{A.12}$$

$$\int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi})\xi^i\xi^j\xi^k\xi^l = \delta^{ijkl} \tag{A.13}$$

$$\int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi})\xi^i\xi^j\xi^k\xi^l\xi^m = 0 \tag{A.14}$$

$$\int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi})\xi^i\xi^j\xi^k\xi^l\xi^m\xi^n = \delta^{ijklmn}. \tag{A.15}$$

$$\vdots$$

$$\int d^D\boldsymbol{\xi}\omega(\boldsymbol{\xi})\xi_\alpha^{i_1}\xi_\alpha^{i_2}\xi_\alpha^{i_3}\ldots\xi_\alpha^{i_M} = \begin{cases} \delta^{i_1 i_2 i_3 \ldots i_M} & \text{if M is even} \\ 0 & \text{if M is odd} \end{cases} \tag{A.16}$$

To illustrate that Eqs.(A.10-A.16) are a consequence of Eq.(A.3) let us consider some examples. The orthogonality of the zeroth and first order Hermite polynomials is,

$$\int d^D\boldsymbol{\xi}\,\omega(\xi)H(\boldsymbol{\xi})H^i(\boldsymbol{\xi}) = \int d^D\boldsymbol{\xi}\,\omega(\xi)\xi^i = 0, \tag{A.17}$$

which yields Eq.(A.10). Integration over two first order Hermite polynomials gives,

$$\int d^D\boldsymbol{\xi}\,\omega(\xi)H^i(\boldsymbol{\xi})H^j(\boldsymbol{\xi}) = \int d^D\boldsymbol{\xi}\,\omega(\xi)\xi^i\xi^j = \delta^{ij}, \tag{A.18}$$

which is Eq.(A.11). Integration over the first and the second order Hermite polynomials gives that,

$$\int d^D\boldsymbol{\xi}\,\omega(\xi)H^i(\boldsymbol{\xi})H^{jk}(\boldsymbol{\xi}) = \int d^D\boldsymbol{\xi}\,\omega(\xi)\xi^i\left(\xi^j\xi^k - \delta^{jk}\right) = 0. \tag{A.19}$$

From Eq.(A.17) one obtains Eq.(A.12). As a last example we consider the integration over two second order Hermite polynomials:

$$\begin{aligned}
&\int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi})H^{ij}(\boldsymbol{\xi})H^{kl}(\boldsymbol{\xi}) = \int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi})[\xi^i\xi^j - \delta^{ij}][\xi^k\xi^l - \delta^{kl}] \\
&= \int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi})\xi^i\xi^j\xi^k\xi^l - \delta^{ij}\int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi})\xi^k\xi^l - \delta^{kl}\int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi})\xi^i\xi^j + \delta^{ij}\delta^{kl}\int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi}) \\
&= \delta^{ik}\delta^{jl} + \delta^{il}\delta^{kj}.
\end{aligned}$$

that gives the Eq.(A.13). The orthogonality relations, given by Eqs.(A.9)-(A.16) are the key ingredients to obtain the moments of Eqs.(3.39), (3.40) and (3.41).

It is worth to investigate the properties of the Hermite polynomials in case the argument is a difference $\xi - u$. Using (A.4), (A.5), (A.6), (A.7) we find the following relations:

$$H^i(\boldsymbol{\xi}) = H^i(\boldsymbol{\xi} - \boldsymbol{u}) + u^i H \tag{A.20}$$

$$H^{ij}(\boldsymbol{\xi}) = H^{ij}(\boldsymbol{\xi} - \boldsymbol{u}) + u^i H^j(\boldsymbol{\xi} - \boldsymbol{u}) + u^j H^i(\boldsymbol{\xi} - \boldsymbol{u}) + u^i u^j H \tag{A.21}$$

$$\begin{aligned}
H^{ijk}(\boldsymbol{\xi}) \;=\; & H^{ijk}(\boldsymbol{\xi} - \boldsymbol{u}) + u^i H^{jk}(\boldsymbol{\xi} - \boldsymbol{u}) \\
& + u^j H^{ik}(\boldsymbol{\xi} - \boldsymbol{u}) + u^k H^{ij}(\boldsymbol{\xi} - \boldsymbol{u}) + u^i u^j H^k(\boldsymbol{\xi} - \boldsymbol{u}) \\
& + u^i u^k H^j(\boldsymbol{\xi} - \boldsymbol{u}) + u^j u^k H^i(\boldsymbol{\xi} - \boldsymbol{u}) + u^i u^j u^k H
\end{aligned} \tag{A.22}$$

$$
\begin{aligned}
H^{ijkl}(\boldsymbol{\xi}) &= H^{ijkl}(\boldsymbol{\xi}-\boldsymbol{u}) + u^i H^{jkl}(\boldsymbol{\xi}-\boldsymbol{u}) \\
&\quad + u^j H^{ikl}(\boldsymbol{\xi}-\boldsymbol{u}) + u^k H^{ijl}(\boldsymbol{\xi}-\boldsymbol{u}) + u^l H^{ijk}(\boldsymbol{\xi}-\boldsymbol{u}) \\
&\quad + u^i u^j H^{kl}(\boldsymbol{\xi}-\boldsymbol{u}) + u^i u^k H^{jl}(\boldsymbol{\xi}-\boldsymbol{u}) + u^i u^l H^{jk}(\boldsymbol{\xi}-\boldsymbol{u}) \\
&\quad + u^k u^l H^{ij}(\boldsymbol{\xi}-\boldsymbol{u}) + u^j u^l H^{ik}(\boldsymbol{\xi}-\boldsymbol{u}) + u^j u^k H^{il}(\boldsymbol{\xi}-\boldsymbol{u}) \\
&\quad + u^i u^j u^k H^{l}(\boldsymbol{\xi}-\boldsymbol{u}) + u^i u^j u^l H^{k}(\boldsymbol{\xi}-\boldsymbol{u}) \\
&\quad + u^j u^k u^l H^{i}(\boldsymbol{\xi}-\boldsymbol{u}) + u^i u^k u^l H^{j}(\boldsymbol{\xi}-\boldsymbol{u}) + u^i u^j u^k u^l. \qquad \text{(A.23)}
\end{aligned}
$$

Using the above expressions it becomes straightforward to calculate the first four coefficients of the Hermite expansion.

Appendix B

Chapman-Enskog assumption and the conservation laws for classical fluid

In this appendix we see how the Chapman Enskog assumption is related to the conservation laws [40]: for mass, momentum and energy. Unlike what was done in chapter 4 to get the conservations laws, here we won't do that in discrete phase space, but in continuous one.

Considering a classical fluid, that obeys Maxwell-Boltzmann distribution for velocities, Eq.(3.33), in three dimensions

$$f^{(0)}(\xi) = \frac{\rho_0}{(2\pi\theta_0)^{3/2}} e^{-(\boldsymbol{\xi}-\boldsymbol{u_0})^2/2\theta_0}, \tag{B.1}$$

where ρ_0, $\boldsymbol{u_0}$ and θ_0 are the density, macroscopic velocity and temperature respectively for the equilibrium state. This notation is used only in this appendix. We can define the density ρ, the macroscopic velocity $\boldsymbol{u}$ and the temperature θ for non-equilibrium state as integrals of distribution function, as follows:

$$\int f d^3\boldsymbol{\xi} \equiv \rho, \tag{B.2}$$

$$\int f \xi^i d^3\boldsymbol{\xi} \equiv \rho u^i, \text{ and} \tag{B.3}$$

$$\int f \boldsymbol{\xi}^2 d^3\boldsymbol{\xi} \equiv \rho \boldsymbol{u}^2 + 3\rho\theta. \tag{B.4}$$

These are the three moments of the non-equilibrium distribution function. The BGK-Boltzmann equation, Eq.(3.20), is

$$\frac{\partial f}{\partial t} + \xi^i \frac{\partial f}{\partial x^i} + F^i \frac{\partial f}{\partial \xi^i} = \frac{1}{\tau}(f^{(0)} - f), \tag{B.5}$$

which we can write as

$$f = f^{(0)} - \tau \left(\frac{\partial f}{\partial t} + \xi^i \frac{\partial f}{\partial x^i} + F^i \frac{\partial f}{\partial \xi^i} \right). \tag{B.6}$$

This expression is used in the following section to get the integrals and derivatives of the distribution function.

Integrating the Maxwell-Boltzmann function, Eq.(B.1) we can get the five moments bellow:

$$\int f^{(0)} d^3\boldsymbol{\xi} = \rho_0, \tag{B.7}$$

$$\int f^{(0)} (\xi^i - u_0^i) d^3\boldsymbol{\xi} = 0, \tag{B.8}$$

$$\int f^{(0)} (\xi^i - u_0^i)(\xi^j - u_0^j) d^3\boldsymbol{\xi} = \rho_0 \theta_0 \delta^{ij}, \tag{B.9}$$

$$\int f^{(0)} (\xi^i - u_0^i)(\xi^j - u_0^j)(\xi^k - u_0^k) d^3\boldsymbol{\xi} = 0, \tag{B.10}$$

$$\int f^{(0)} (\xi^i - u_0^i)(\xi^j - u_0^j)(\boldsymbol{\xi} - \boldsymbol{u_0})^2 d^3\boldsymbol{\xi} = 5\rho_0 \theta_0^2 \delta^{ij}. \tag{B.11}$$

This notation is used only in this appendix.

B.1 Conservation of mass

Integrating the equation (B.5)

$$\frac{\partial}{\partial t} \int f d^3\boldsymbol{\xi} + \frac{\partial}{\partial x^i} \int f u^i d^3\boldsymbol{\xi} + F^i \int \frac{\partial f}{\partial \xi^i} d^3\boldsymbol{\xi} = \frac{1}{\tau} \int (f^{(0)} - f) d^3\boldsymbol{\xi}. \tag{B.12}$$

The first and second integrals are given by Eqs.(B.2) and (B.3), and the integral $\int \partial f/\partial \xi^i d^3\boldsymbol{\xi} = 0$, because the distribution function is odd and the integral is defined over all velocity space. Now, we use the *first Chapmann-Enskog assumption*: ρ is equal to ρ_0. Comparing Eq.(B.7) and (B.2), we conclude

$$\int f d^3\boldsymbol{\xi} = \int f^{(0)} d^3\boldsymbol{\xi} \Rightarrow \int (f^{(0)} - f) d^3\boldsymbol{\xi} = 0. \tag{B.13}$$

It is a necessary condition to obtain the correct law for conservation of mass given in Eq.(2.3):

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x^i}(\rho u^i) = 0. \tag{B.14}$$

B.2 Conservation of momentum

Integrating the Eq.(B.5) multiplied by ξ^i, we get

$$\frac{\partial}{\partial t}\int f\xi^i d^3\boldsymbol{\xi} + \frac{\partial}{\partial x^j}\int f\xi^i\xi^j d^3\boldsymbol{\xi} + F^j \int \frac{\partial f}{\partial \xi^j}\xi^i d^3\boldsymbol{\xi} = \frac{1}{\tau}\int (f^{(0)} - f)\xi^i d^3\boldsymbol{\xi} \tag{B.15}$$

Now we need call the *second Chapmann-Enskog assumption*, that is, $\boldsymbol{u} = \boldsymbol{u_0}$. Eqs.(B.3) and (B.8) give

$$\int f\xi^i d^3\boldsymbol{\xi} = \int f^{(0)}\xi^i d^3\boldsymbol{\xi} \Rightarrow \int (f^{(0)} - f)\xi^i d^3\boldsymbol{\xi} = 0. \tag{B.16}$$

As we see in the end of this calculation, we obtain the momentum conservation equation only because this integral is zero. The third integral can be solved

$$\int \frac{\partial f}{\partial \xi^j}\xi^i d^3\boldsymbol{\xi} = \int \frac{\partial}{\partial \xi^j}(f\xi^i) d^3\boldsymbol{\xi} - \int f\frac{\partial \xi^i}{\partial \xi^j} d^3\boldsymbol{\xi} = 0 - \delta^{ij}\int f d^3\boldsymbol{\xi} = -n\delta^{ij}, \tag{B.17}$$

where the integral $\int \partial(f\xi^i)/\partial\xi^j d^3\boldsymbol{\xi}$ was zero because the function $f\xi^i$ is odd. Thus, using these results and Eq.(B.3), we have that Eq.(B.15) becomes

$$\frac{\partial}{\partial t}(\rho u^i) + \frac{\partial}{\partial x^j}\int f\xi^i\xi^j d^3\boldsymbol{\xi} - F^i\rho = 0. \tag{B.18}$$

Now we need to find the remaining integral. Substituting Eq.(B.6) into the integral,

$$\int f\xi^i\xi^j d^3\boldsymbol{\xi} = \int f^{(0)}\xi^i\xi^j d^3\boldsymbol{\xi} - \tau\left(\frac{\partial}{\partial t}\int f\xi^i\xi^j d^3\boldsymbol{\xi} + \frac{\partial}{\partial x^k}\int f\xi^i\xi^j\xi^k d^3\boldsymbol{\xi} + \rho F^i u^j + \rho u^i F^j\right) + O(\partial^2). \tag{B.19}$$

So, considering only first order in derivatives, Eq.(B.15) is the Euler equation given by Eq.(2.5):

$$\frac{\partial}{\partial t}(\rho u^i) + \frac{\partial}{\partial x^j}(\rho u^i u^j) = -\frac{\partial}{\partial x^i}(\rho\theta) + \rho F^i. \tag{B.20}$$

But we can find this equation in higher order by solving the integrals in equation (B.19). From third moment of equilibrium function, Eq.(B.9), we get $\int f^{(0)}\xi^i\xi^j d^3\boldsymbol{\xi} = \rho u^i u^j + \rho\theta\delta^{ij}$. Taking the time derivative and using Eqs.(B.20) and (B.14),

$$\begin{aligned}\frac{\partial}{\partial t}\int f^{(0)}\xi^i\xi^j d^3\boldsymbol{\xi} &= -\frac{\partial}{\partial x^k}(\rho u^i u^k)u^j - \frac{\partial}{\partial x^i}(\rho\theta)u^j + \rho F^i u^j - \rho u^i u^k\frac{\partial u^j}{\partial x^k} \\ &\quad -u^i\frac{\partial}{\partial x^j}(\rho\theta) - \rho F^j u^i - \frac{\partial}{\partial x^k}(\rho\theta u^k)\delta^{ij} - \frac{2}{3}\rho\theta\frac{\partial u^k}{\partial x^k}\delta^{ij}.\end{aligned} \tag{B.21}$$

Using Eq.(B.10) and deriving

$$\begin{aligned}&\frac{\partial}{\partial x^k}\int f^{(0)}\xi^i\xi^j\xi^k d^3\boldsymbol{\xi} \\ &= \delta^{ik}\frac{\partial}{\partial x^k}(\rho\theta u^j) + \delta^{jk}\frac{\partial}{\partial x^k}(\rho\theta u^i) + \delta^{ij}\frac{\partial}{\partial x^k}(\rho\theta u^k) - \frac{\partial}{\partial x^k}(\rho u^i u^j u^k) \\ &= \frac{\partial}{\partial x^i}(\rho\theta u^j) + \frac{\partial}{\partial x^j}(\rho\theta u^i) + \frac{\partial}{\partial x^k}(\rho\theta u^k)\delta^{ij} - \frac{\partial}{\partial x^k}(\rho u^i u^j u^k).\end{aligned} \tag{B.22}$$

The sum of the two above integrals, after arrangement, is

$$\begin{aligned}&\frac{\partial}{\partial t}\int f^{(0)}\xi^i\xi^j d^3\boldsymbol{\xi} + \frac{\partial}{\partial x^k}\int f^{(0)}\xi^i\xi^j\xi^k d^3\boldsymbol{\xi} \\ &= \rho\theta\frac{\partial u^i}{\partial x^j} + \rho\theta\frac{\partial u^j}{\partial x^i} - \frac{2}{3}\rho\theta\frac{\partial u^k}{\partial x^k}\delta^{ij} - \rho F^i u^j - \rho F^j u^i.\end{aligned} \tag{B.23}$$

Substituting this result in Eq.(B.19),

$$\int f\xi^i\xi^j d^3\boldsymbol{\xi} = \rho\theta\delta^{ij} + \rho u^i u^j - \tau\rho\theta\frac{\partial u^j}{\partial x^i} - \tau\rho\theta\frac{\partial u^i}{\partial x^j} + \frac{2}{3}\tau\rho\theta\frac{\partial u^k}{\partial x^k}\delta^{ij} \tag{B.24}$$

Finally,

$$\rho\frac{\partial u^i}{\partial t}+\rho u^j\frac{\partial u^i}{\partial x^j}=-\frac{\partial}{\partial x^i}(\rho\theta)+\rho F^i+\frac{\partial}{\partial x^j}\left[\tau\rho\theta\left(\frac{\partial u^j}{\partial x^i}+\frac{\partial u^i}{\partial x^j}-\frac{2}{3}\frac{\partial u^k}{\partial x^k}\delta^{ij}\right)\right] \quad \text{(B.25)}$$

This is the Navier-Stokes equation that is in Eq.(2.25). We see that this result could be obtained only because we assumed the second Chapmann-Enskog assumption.

B.3 Conservation of energy

Multiplying Eq.(B.5) by $(\boldsymbol{\xi}-\boldsymbol{u})^2$ and integrating, we have

$$\begin{aligned}&\int\frac{\partial f}{\partial t}(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}+\int\xi^i\frac{\partial f}{\partial x^i}(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}\\&+\int F^i\frac{\partial f}{\partial\xi^i}(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}=\frac{1}{\tau}\int(f^{(0)}-f)(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}.\end{aligned} \quad \text{(B.26)}$$

We call the *third Chapmann-Enskog assumption*, i.e., $\theta=\theta_0$. Using Eqs.(B.4) and (B.9), we get

$$\int f(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}=\int f^{(0)}(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}\Rightarrow\int(f^{(0)}-f)(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}=0. \quad \text{(B.27)}$$

Thus,

$$\int\frac{\partial f}{\partial t}(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}+\int\xi^i\frac{\partial f}{\partial x^i}(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}+\int F^i\frac{\partial f}{\partial\xi^i}(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}=0. \quad \text{(B.28)}$$

Now we will solve these integrals. The last integral is

$$\int\frac{\partial f}{\partial\xi^i}(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}=\frac{\partial}{\partial\xi^i}\int f(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}-2\int f(\xi^i-u^i)d^3\boldsymbol{\xi},$$

using Eqs.(B.3) and (B.4),

$$\int\frac{\partial f}{\partial\xi^i}(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}=\frac{\partial}{\partial\xi^i}(3\rho\theta)-0=0. \quad \text{(B.29)}$$

The first integral in Eq.(B.28) gives

$$\int\frac{\partial f}{\partial t}(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}=\frac{\partial}{\partial t}\int f(\boldsymbol{\xi}-\boldsymbol{u})^2d^3\boldsymbol{\xi}+2\frac{\partial\boldsymbol{u}}{\partial t}\cdot\int f(\boldsymbol{\xi}-\boldsymbol{u})d^3\boldsymbol{\xi}=\frac{\partial}{\partial t}(3\rho\theta), \quad \text{(B.30)}$$

where was used Eqs.(B.3) and (B.4). And the remaining integral

$$\begin{aligned}
&\int \xi^i \frac{\partial f}{\partial x^i}(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} = \frac{\partial}{\partial x^i}\int f\xi^i(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} + 2\int f\xi^i(\xi^j-u^j)\frac{\partial u^j}{\partial x^i}d^3\boldsymbol{\xi} \\
= \;& \frac{\partial}{\partial x^i}\int f\xi^i(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} + 2\rho\theta\frac{\partial u^i}{\partial x^i} - \tau\left[\int \frac{\partial f}{\partial t}(\xi^i-u^i)(\xi^j-u^j)d^3\boldsymbol{\xi}\right. \\
& \left. + \int \xi^k\frac{\partial f}{\partial x^k}(\xi^i-u^i)(\xi^j-u^j)d^3\boldsymbol{\xi}\right]\frac{\partial u^j}{\partial x^i} \\
= \;& \frac{\partial}{\partial x^i}\int f\xi^i(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} + 2\rho\theta\frac{\partial u^i}{\partial x^i} - \tau\frac{\partial u^j}{\partial x^i}\left(\frac{\partial u^j}{\partial x^i}+\frac{\partial u^i}{\partial x^j}-\frac{2}{3}\frac{\partial u^k}{\partial x^k}\delta^{ij}\right) \qquad \text{(B.31)}
\end{aligned}$$

And approximating the integral

$$\begin{aligned}
&\int f\xi^i(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} \\
= \;& \int f^{(0)}\xi^i(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} - \tau\left[\int \frac{\partial f}{\partial t}\xi^i(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi}\right. \\
& \left. + \int \frac{\partial f}{\partial x^j}\xi^i\xi^j(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} + F^j\int \frac{\partial f}{\partial \xi^j}\xi^i(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi}\right] \\
= \;& 3\rho\theta u^i - \tau\left[\int \frac{\partial f^{(0)}}{\partial t}\xi^i(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi}\right. \\
& \left. + \int \frac{\partial f^{(0)}}{\partial x^j}\xi^i\xi^j(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} - 5\rho\theta F^i\right] + O(\partial^2). \qquad \text{(B.32)}
\end{aligned}$$

Thus, substituting these results in Eq.(B.28) we have

$$\begin{aligned}
&3\frac{\partial}{\partial t}(\rho\theta) + \frac{\partial}{\partial x^i}\int f\xi^i(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} + 2\rho\theta\frac{\partial u^i}{\partial x^i} \\
&-\tau\frac{\partial u^j}{\partial x^i}\left(\frac{\partial u^j}{\partial x^i}+\frac{\partial u^i}{\partial x^j}-\frac{2}{3}\frac{\partial u^k}{\partial x^k}\delta^{ij}\right) = 0, \qquad \text{(B.33)}
\end{aligned}$$

from which we can write the conservation law in zeroth order:

$$\frac{\partial\theta}{\partial t} + u^i\frac{\partial\theta}{\partial x^i} = -\frac{2}{3}\theta\frac{\partial u^i}{\partial x^i} + O(\partial^2). \qquad \text{(B.34)}$$

If we want a higher order approximation, we need to solve the integrals in (B.32),

$$\begin{aligned}
&\int \frac{\partial f^{(0)}}{\partial t}\xi^i(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} \\
= \;& \frac{\partial}{\partial t}\int f^{(0)}\xi^i(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} + 2\int f^{(0)}\xi^i(\boldsymbol{\xi}-\boldsymbol{u})\cdot\frac{\partial \boldsymbol{u}}{\partial t}d^3\boldsymbol{\xi} \\
= \;& 3\frac{\partial}{\partial t}(\rho\theta u^i) + 2\frac{\partial u^k}{\partial t}\left[\rho\theta\delta^{ik} - u^i\int f^{(0)}(\xi^k-u^k)d^3\boldsymbol{\xi}\right] \\
= \;& 3\frac{\partial}{\partial t}(\rho\theta u^i) + 2\rho\theta\frac{\partial u^i}{\partial t} \\
= \;& 3\theta\left[-\frac{\partial(\rho\theta)}{\partial x^i} + \rho F^i - \frac{\partial}{\partial x^j}(\rho u^i u^j)\right] + 3\rho u^i\left[-\frac{2}{3}\theta\frac{\partial u^j}{\partial x^j} - u^j\frac{\partial\theta}{\partial x^j}\right] \\
& +2\rho\theta\left[-\frac{1}{\rho}\frac{\partial}{\partial x^i}(\rho\theta) - u^j\frac{\partial u^i}{\partial x^j} + F^i\right] \\
= \;& \frac{\partial}{\partial x^j}(-3\theta\rho u^i u^j) - 2\rho\theta\frac{\partial}{\partial x^j}(u^i u^j) - 5\theta\frac{\partial}{\partial x^i}(\rho\theta) + 5\rho F^i. \qquad \text{(B.35)}
\end{aligned}$$

The other integral is

$$\begin{aligned}
\int \frac{\partial f^{(0)}}{\partial x^j}\xi^i\xi^j(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} \;=\; & \frac{\partial}{\partial x^j}\int f^{(0)}\xi^i\xi^j(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} \\
& +2\int f^{(0)}\xi^i\xi^j(\boldsymbol{\xi}-\boldsymbol{u})\cdot\frac{\partial \boldsymbol{u}}{\partial x^j}, \qquad \text{(B.36)}
\end{aligned}$$

but, from Eq.(B.11)

$$\begin{aligned}
&\int(\xi^i-u^i)(\xi^j-u^j)(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} = 5\rho\theta^2\delta^{ij} \\
= \;& \int f^{(0)}\xi^i\xi^j(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} - u^j\int f^{(0)}\xi^i(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} \\
& -u^i\int f^{(0)}\xi^j(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} + u^i u^j\int f^{(0)}(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} \qquad \text{(B.37)}
\end{aligned}$$

$$\Rightarrow \int f^{(0)}\xi^i\xi^j(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} = 5\rho\theta^2\delta^{ij} + 3u^i u^j\rho\theta. \qquad \text{(B.38)}$$

We also have, Eq.(B.10)

$$\int f^{(0)}(\xi^i-u^i)(\xi^j-u^j)(\xi^k-u^k)d^3\boldsymbol{\xi} = 0 \qquad \text{(B.39)}$$

$$\Rightarrow \int f^{(0)}\xi^i\xi^j(\xi^k-u^k)d^3\boldsymbol{\xi} = \rho\theta(u^j\delta^{ik} + u^i\delta^{jk}). \qquad \text{(B.40)}$$

Thus

$$\int \frac{\partial f^{(0)}}{\partial x^j}\xi^i\xi^j(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} = \frac{\partial}{\partial x^i}(5\rho\theta^2) + \frac{\partial}{\partial x^j}(3u^iu^j\rho\theta) + 2\rho\theta\frac{\partial}{\partial x^j}(u^iu^j). \tag{B.41}$$

Substituting

$$\begin{aligned}
&\int f\xi^i(\boldsymbol{\xi}-\boldsymbol{u})^2 d^3\boldsymbol{\xi} \\
= \;& 3\rho\theta u^i - \tau\left[\frac{\partial}{\partial x^j}(-3\theta\rho u^iu^j) - 2\rho\theta\frac{\partial}{\partial x^j}(u^iu^j) - 5\theta\frac{\partial}{\partial x^i}(\rho\theta) + 5\rho F^i\right. \\
& \left. + \frac{\partial}{\partial x^i}(5\rho\theta^2) + \frac{\partial}{\partial x^j}(3\rho\theta u^iu^j) + 2\rho\theta\frac{\partial}{\partial x^j}(u^iu^j) - 5\rho\theta F^i\right] \\
= \;& 3\rho\theta u^i - \tau\left[5\rho\theta\frac{\partial\theta}{\partial x^i} + 5\rho F^i - 5\rho\theta F^i\right],
\end{aligned} \tag{B.42}$$

and we finally obtain the equation for energy conservation (see Eq.(2.29))

$$\frac{\partial\theta}{\partial t} + u^i\frac{\partial\theta}{\partial x^i} = -\frac{2}{3}\theta\frac{\partial u^i}{\partial x^i} + \frac{1}{\rho}\frac{\partial}{\partial x^i}\left(\frac{5\rho\theta}{3}\frac{\partial\theta}{\partial x^i}\right) + \tau\frac{\partial u^j}{\partial x^i}\left(\frac{\partial u^j}{\partial x^i} + \frac{\partial u^i}{\partial x^j} - \frac{2}{3}\frac{\partial u^k}{\partial x^k}\delta^{ij}\right). \tag{B.43}$$

Again, we get this result because we assumed the third Chapmann-Enskog assumption.

We can see by these previous calculations that the Chapmann-Enskog assumptions are closely related to the correct achievement of the correct hydrodynamic laws.

Appendix C

Gauss-Hermite quadrature

I review the Gauss-Hermite quadrature, which is a way to obtain the values of integrals through discrete sums. In this way we transform our equilibrium distribution functions obtained in the previous section in a LBM scheme to numerically solve the BGK-Boltzmann equation. The Gauss-Hermite quadrature preserves the orthogonality of the Hermite polynomial tensors in the Hilbert space [24]. Then the gaussian integrals can be performed in a D-dimensional *discrete* space where the microscopic velocity only takes the fixed set of values, $\boldsymbol{\xi}_\alpha$, $\alpha = 0, 1, \cdots, M_\alpha - 1$, provided that we introduce the set of weights w_α. Essentially this means that the gaussian integral over an arbitrary function $G(\boldsymbol{\xi})$ can be performed as a sum over a set of M_α velocities:

$$\int d^D\boldsymbol{\xi}\, \omega(\boldsymbol{\xi}) G(\boldsymbol{\xi}) = \sum_\alpha w_\alpha G(\boldsymbol{\xi}_\alpha)\,. \tag{C.1}$$

Thus the orthonormality condition of the Hermite polynomials, shown in Eq.(A.3), also holds in this discrete space:

$$\begin{aligned} &\sum_\alpha w_\alpha H^{i_1 i_2 \ldots i_N}(\boldsymbol{\xi}_\alpha) H^{j_1 j_2 \ldots j_M}(\boldsymbol{\xi}_\alpha) \\ &= \delta^{NM}(\delta^{i_1 j_1}\delta^{i_2 j_2}\ldots\delta^{i_N j_N} + \text{all permutations of j's}) \end{aligned} \tag{C.2}$$

Notice the two distinct integers, the truncation order of the Hermite expansion of the equilibrium distribution, N, and also M, where M is the number of relations that the discrete set of velocities and weights w_α must satisfy [24]. In section 3.3 we saw these relations, that are Eqs.(3.52)-(3.59) and replace the continuum Eqs. (A.9)-(A.16).

Lattice	M	ξ_α	w_α
D1V2	3	± 1	$1/2$
D1V3	5	0	$2/3$
		$\pm\sqrt{3}$	$1/6$
D1V4	7	$\pm\sqrt{3-\sqrt{6}}$	$(3+\sqrt{6})/12$
		$\pm\sqrt{3+\sqrt{6}}$	$(3-\sqrt{6})/12$
D1V5	9	0	$8/15$
		$\pm\sqrt{5-\sqrt{10}}$	$(7+2\sqrt{10})/60$
		$\pm\sqrt{5+\sqrt{10}}$	$(7-2\sqrt{10})/60$

Table C.1: One-dimension lattices and their weights. M is the number of relations that the lattice must satisfy.

Lattice	M	ξ_α	p	w_α	
D2V6	4	$(0,0)$	1	$1/2$	
		$2\left(\cos\frac{2\pi n}{5}, \sin\frac{2\pi n}{5}\right)$	5	$1/10$	$n=1,\ldots,5$
D2V7	5	$(0,0)$	1	$1/2$	
		$2\left(\cos\frac{n\pi}{3}, \sin\frac{n\pi}{3}\right)$	6	$1/12$	$n=1,\ldots,6$
D2V9	5	$(0,0)$	1	$4/9$	
		$(\sqrt{3},0)_{FS}$	4	$1/9$	
		$(\pm\sqrt{3},\pm\sqrt{3})$	4	$1/36$	
D2V12	7	$(r,0)_{FS}$	4	$1/36$	$r^2=6$
		$(\pm s,\pm s)$	4	$(5+2\sqrt{5})/45$	$s^2=(9-3\sqrt{5})/4$
		$(\pm t,\pm t)$	4	$(5-2\sqrt{5})/45$	$t^2=(9+3\sqrt{5})/4$
D2V17	7	$(0,0)$	1	$(575+193\sqrt{193})/8100$	
		$(r,0)_{FS}$	4	$(3355-91\sqrt{193})/18000$	$r^2=\frac{(125+5\sqrt{193})}{72}$
		$(\pm r,\pm r)$	4	$(655+17\sqrt{193})/27000$	
		$(\pm 2r,\pm 2r)$	4	$(685-49\sqrt{193})/54000$	
		$(3r,0)_{FS}$	4	$(1445-101\sqrt{193})/162000$	

Table C.2: Two-dimension lattices and their weights. M is the number of relations that the lattice must satisfy and p is the number of velocities with the coordinates in the same line. The subscript FS denotes a fully symmetric set of points.

ξ_α	p	w_α
$(0,0)$	1	$\frac{56266R^2-7^{2/3}(19991-338\sqrt{30})R+7^{4/3}(14323+6238\sqrt{30})}{264600R^2}$
$(a,0)_{FS}$	4	$\frac{31206R^2-7^{2/3}(3201+466\sqrt{30})R-7^{4/3}(2427-706\sqrt{30})}{264600R^2}$
$(\pm a,\pm a)$	4	$\frac{29232R^2+7^{2/3}(3888+265\sqrt{30})R+7^{4/3}(216-1027\sqrt{30})}{529200R^2}$
$(2a,0)_{FS}$	4	$\frac{42R^2+7^{2/3}(33+2\sqrt{30})R-7^{1/3}(3+62\sqrt{30})}{3600R^2}$
$(\pm a,\pm 2a)_{FS}$	8	$\frac{1638R^2+7^{2/3}(1647+4\sqrt{30})R-7^{4/3}(891+496\sqrt{30})}{264600R^2}$
$(\pm 2a,\pm 2a)$	4	$\frac{-126R^2+7^{2/3}(1161+194\sqrt{30})R+7^{4/3}(1107-242\sqrt{30})}{1058400R^2}$
$(3,0)_{FS}$	4	$\frac{14R^2+7^{2/3}(131+10\sqrt{30})R+7^{4/3}(17-34\sqrt{30})}{264600R^2}$
$(\pm a,\pm 3a)_{FS}$	8	$\frac{-168R^2+7^{2/3}(228+71\sqrt{30})R+7^{4/3}(516-29\sqrt{30})}{1058400R^2}$
$R=\sqrt[3]{67+36\sqrt{30}}$		$a=\frac{1}{6}\sqrt{49-\frac{17.(7)^{2/3}}{R}+7^{1/3}R}$

Table C.3: D2V37 lattice. It has $M = 9$. The subscript FS denotes a fully symmetric set of points.

Lattice	M	ξ_α	p	w_α	
D3V13	5	$(0,0,0)$	1	$2/5$	
		$(\pm r,\pm s,0)$	4	$1/20$	$r^2=(5+\sqrt{5})/2$
		$(0,\pm r,\pm s)$	4	$1/20$	$s^2=(5-\sqrt{5})/2$
		$(\pm s,0,\pm r)$	4	$1/20$	
D3V15	5	$(0,0,0)$	1	$2/9$	
		$(\sqrt{3},0,0)_{FS}$	6	$1/9$	
		$(\pm\sqrt{3},\pm\sqrt{3},\pm\sqrt{3})$	8	$1/72$	
D3V19	5	$(0,0,0)$	1	$1/3$	
		$(\sqrt{3},0,0)_{FS}$	6	$1/18$	
		$(\sqrt{3},\sqrt{3},0)_{FS}$	12	$1/36$	
D3V27	5	$(0,0,0)$	1	$8/27$	
		$(\sqrt{3},0,0)_{FS}$	6	$2/27$	
		$(\sqrt{3},\sqrt{3},0)_{FS}$	12	$1/54$	
		$(\pm\sqrt{3},\pm\sqrt{3},\pm\sqrt{3})$	8	$1/216$	

Table C.4: Three-dimension lattices and their weights. M is the number of relations that the lattice must satisfy and p is the number of velocities with the coordinates in the same line. The subscript FS denotes a fully symmetric set of points.

Appendix D

Useful relations

$$\sum_\alpha \xi_\alpha^i \xi_\alpha^j \xi_\alpha^k \xi_\alpha^k w_\alpha = (D+2)\delta^{ij} \tag{D.1}$$

$$\sum_\alpha \xi_\alpha^i \xi_\alpha^j (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u})^2 w_\alpha = \boldsymbol{u}^2 \delta^{ij} + 2u^i u^j \tag{D.2}$$

$$\sum_\alpha \xi_\alpha^i \xi_\alpha^j (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u})^4 w_\alpha = 3\boldsymbol{u}^4 \delta^{ij} + 12\boldsymbol{u}^2 u^i u^j \tag{D.3}$$

$$\sum_\alpha \xi_\alpha^i \xi_\alpha^j (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u})^2 \boldsymbol{\xi_\alpha}^2 w_\alpha = u^i u^j (2D+8) + \delta^{ij}(D+4)\boldsymbol{u}^2 \tag{D.4}$$

$$\sum_\alpha \xi_\alpha^i \xi_\alpha^j \boldsymbol{\xi_\alpha}^4 w_\alpha = \delta^{ij}(D^2+6D+8) \tag{D.5}$$

$$\sum_\alpha \xi_\alpha^i \xi_\alpha^j \xi_\alpha^k (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u}) w_\alpha = u^k \delta^{ij} + u^j \delta^{ik} + u^i \delta^{jk} \tag{D.6}$$

$$\sum_\alpha \xi_\alpha^i \xi_\alpha^j \xi_\alpha^k (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u})^3 w_\alpha = 3(u^k \delta^{ij} + u^j \delta^{ik} + u^i \delta^{jk})\boldsymbol{u}^2 + 6u^i u^j u^k \tag{D.7}$$

$$\sum_\alpha \xi_\alpha^i \xi_\alpha^j \xi_\alpha^k (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u}) \boldsymbol{\xi_\alpha}^2 w_\alpha = (D+4)(u^k \delta^{ij} + u^j \delta^{ik} + u^i \delta^{jk}) \tag{D.8}$$

$$\sum_\alpha \boldsymbol{\xi_\alpha}^2 w_\alpha = D \tag{D.9}$$

$$\sum_\alpha \boldsymbol{\xi_\alpha}^2 (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u})^2 w_\alpha = (D+2)\boldsymbol{u}^2 \tag{D.10}$$

$$\sum_\alpha \boldsymbol{\xi_\alpha}^2 (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u})^4 w_\alpha = 3(D+4)\boldsymbol{u}^4 \tag{D.11}$$

$$\sum_\alpha \boldsymbol{\xi_\alpha}^4 w_\alpha = D(D+2) \tag{D.12}$$

$$\sum_\alpha {\boldsymbol{\xi_\alpha}}^4 (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u})^2 w_\alpha = (D+2)(D+4)\boldsymbol{u}^2 \tag{D.13}$$

$$\sum_\alpha {\boldsymbol{\xi_\alpha}}^6 w_\alpha = D^3 + 6D^2 + 8D \tag{D.14}$$

$$\sum_\alpha {\boldsymbol{\xi_\alpha}}^2 \xi_\alpha^i (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u}) w_\alpha = (D+2)u^j \tag{D.15}$$

$$\sum_\alpha {\boldsymbol{\xi_\alpha}}^2 \xi_\alpha^j (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u})^3 w_\alpha = 3(D+4)u^j \boldsymbol{u}^2 \tag{D.16}$$

$$\sum_\alpha {\boldsymbol{\xi_\alpha}}^4 \xi_\alpha^j (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u}) w_\alpha = (D+4)(D+2)u^j \tag{D.17}$$

$$\sum_\alpha {\boldsymbol{\xi_\alpha}}^2 \xi_\alpha^j \xi_\alpha^k (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u})^4 w_\alpha = 3(D+6)(\boldsymbol{u}^4 \delta^{jk} + 4u^j u^k \boldsymbol{u}^2) \tag{D.18}$$

$$\sum_\alpha {\boldsymbol{\xi_\alpha}}^4 \xi_\alpha^j \xi_\alpha^k (\boldsymbol{\xi_\alpha} \cdot \boldsymbol{u})^2 w_\alpha = (D+4)(D+6)(\boldsymbol{u}^2 \delta^{jk} + 2u^j u^k) \tag{D.19}$$

$$\sum_\alpha {\boldsymbol{\xi_\alpha}}^6 \xi_\alpha^j \xi_\alpha^k w_\alpha = (D+2)(D+4)(D+6)\delta^{jk} \tag{D.20}$$