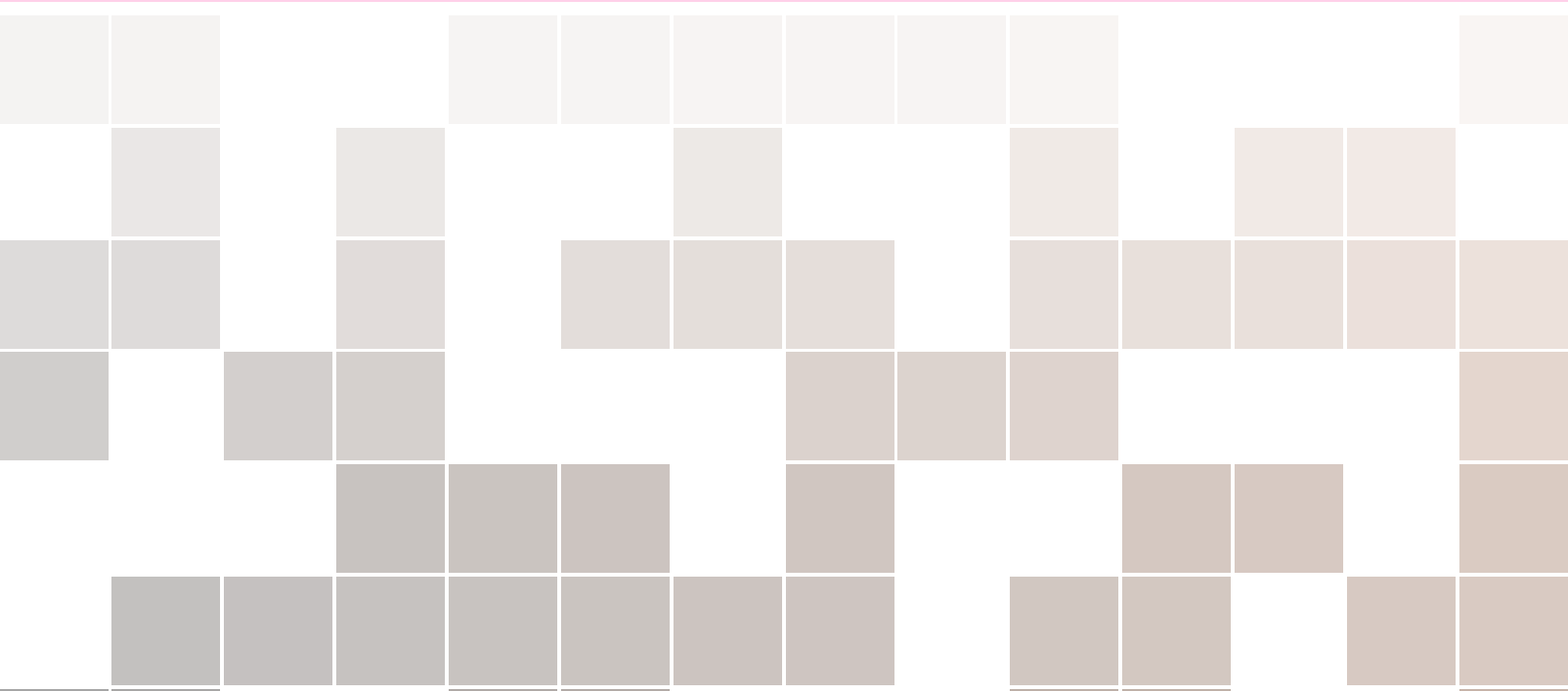


Lattice Boltzmann Method From Beginners to Researchers

Edition 0.1

By the **LatticeX** Project



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For Beginners

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Chapter 1 Background Knowledge

1.1 Mathematical Notations

1.1.1 Index Notation versus Vector Notation

Index notation (a.k.a. Cartesian notation) is a powerful tool for manipulating multidimensional equations. However, there are times when the more conventional vector notation is more useful. It is therefore important to be able to easily convert back and forth between the two. This primer will use both index and vector formulations, and will adhere to the notation conventions summarized below:

Table 1.1: Notations

	tensor notation	index notation
scalar	a	a
vector	\mathbf{a}	a_α
tensor	\mathbf{a}	$a_{\alpha\beta}$

In either notation, we tend to group quantities into one of three categories:

- **scalar** A magnitude that does not change with a rotation of axes.
- **vector** Associates a scalar with a direction.
- **tensor** Associates a vector (or tensor) with a direction.

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- **scalar** A magnitude that does not change with a rotation of axes.
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A scalar is any physical property which can be represented by a single real number in some chosen unit system, e.g. pressure ($\text{kg}\cdot\text{m}^{-1}\cdot\text{s}^{-2}$), temperature (K) and density ($\text{kg}\cdot\text{m}^{-3}$). Scalars are denoted by single letters in italics, e.g. p , T , ρ . The standard scalar operations (addition, subtraction and equality) are only physically meaningful for scalars of the same dimensional units, i.e. standard scalar operations must be performed using consistent units of measurement.

A vector is an entity which is represented by both magnitude and direction. In its most general form an n -dimensional vector \mathbf{a} can be denoted by n scalar components (a_1, a_2, \dots, a_n) corresponding to coordinate axes x_1, x_2, \dots, x_n (or measured with respect to these coordinate axes). For continuum mechanics, where we deal with 3 dimensional (Euclidean) space, the vector $\mathbf{a} = (a_1, a_2, a_3)$ relates to a general set of axes x_1, x_2, x_3 ; representing x, y, z in a **Cartesian coordinate system**, or r, θ, z in **cylindrical coordinate system**, or r, θ, ϕ in **spherical coordinate system**.

The index notation presents the same vector as $a_i (i = 1, 2, \dots, n)$ in which i corresponds to each of the coordinate axes. The list of indices $(i = 1, 2, \dots, n)$ is usually omitted in mathematical text since it is implied by the form of the equation in which it is written. In this article the tensor notation will generally be used in which a vector or tensor is represented by letters in bold face, e.g. \mathbf{a} . The benefits of this notation are that: it does not imply anything about the coordinate system; it therefore promotes the concept of a vector as an entity with direction and magnitude rather than a group of three scalars; and, it is more compact.

The magnitude, or modulus of a vector \mathbf{a} or a_i is denoted by $|\mathbf{a}|$ and a in respective notations. Vectors of unit magnitude are referred to as unit vectors. It is assumed that the reader is familiar with the basic operations of multiplication of a vector and scalar and vector addition and subtraction, which are both commutative and associative. The next three sections describe the remaining vector and tensor operations required in continuum mechanics.

A strength of index notation is that it allows the use of the *Einstein summation convention* where repeating the same index twice in a single term implies summation over all possible values of that index. Thus, the dot product of two n -dimensional vectors a_i and b_i can be expressed as [1]

$$a_i b_i = \sum_{i=1}^n a_i b_i = \mathbf{a} \cdot \mathbf{b} = a_1 b_1 + a_2 b_2 + \cdots + a_n b_n \quad (1.1)$$

For the dyadic product,

$$\mathbf{A} = \mathbf{a} \otimes \mathbf{b} \Leftrightarrow A_{\alpha\beta} = a_\alpha b_\beta \quad (1.2)$$

There are several equivalent terms and notations for dyadic product: Dyadic, outer, and tensor products [2, 3]:

1. The **dyadic product** of two vectors \mathbf{a} and \mathbf{b} is denoted by \mathbf{ab} (no symbol; no multiplication signs, crosses, dots etc.)
2. The **outer product** of two column vectors \mathbf{a} and \mathbf{b} is denoted and defined as $\mathbf{a} \otimes \mathbf{b}$ or \mathbf{ab}^T , where T means transpose.
3. The **tensor product** of two vectors \mathbf{a} and \mathbf{b} is denoted $\mathbf{a} \otimes \mathbf{b}$.

In the dyadic context they all have the same definition and meaning, and are used synonymously, although the tensor product is an instance of the more general and abstract use of the term.

1.1.2 Notations in Current Book

Throughout this book we utilize the index notation, using Greek indices to denote an arbitrary component of a vector or a tensor, e.g. $f_\alpha \in \{f_x, f_y, f_z\}$.

We may also use index notation to generalize coordinate notation: a general component of the spatial coordinate vector $\mathbf{r} = (x, y, z)$ can be written α . In this way, we can also express, e.g., gradients in index notation:

$$\nabla \lambda(\mathbf{r}) \Leftrightarrow \frac{\partial \lambda(\mathbf{r})}{\partial \mathbf{r}} = \frac{\partial \lambda(\mathbf{r})}{\partial \alpha} = \partial_\alpha \lambda(\mathbf{r}) \quad (1.3)$$

in which, $\frac{\partial}{\partial \mathbf{r}} = \nabla = \mathbf{e}_x \frac{\partial}{\partial x} + \mathbf{e}_y \frac{\partial}{\partial y} + \mathbf{e}_z \frac{\partial}{\partial z} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$ [4].

The third option is a common shorthand notation for derivatives, used throughout the literature and this book. Similarly, the time derivative can be expressed using the shorthand notation $\frac{\partial \lambda(t)}{\partial t} = \partial_t \lambda(t)$.

In this book, we use Greek indices for the Cartesian indices x , y , and z . We also use Roman indices such as i , j , and k for non-Cartesian indices, typically to index discrete velocities as e.g. ξ_i . Einstein's summation convention is used only for the Cartesian indices.

1.1.3 Common Operations

To be continue ...

1.2 Conservation Laws of Fluid Motion

1.2.1 Governing Equations of Fluid Flow

1.2.1.1 Mass Conservation in Three Dimensions

1.2.1.2 Rates of Change Following a Fluid Particle

In continuum mechanics, the material derivative describes the time rate of change of some physical quantity (like heat or momentum) of a material element that is subjected to space-and-time-dependent macroscopic velocity field variations of that physical quantity. The material derivative can serve as a link between Eulerian and Lagrangian descriptions of continuum deformation.

There are many other names for the material derivative, including: advective derivative, convective derivative, derivative following the motion, Lagrangian derivative, particle derivative, substantial derivative, substantive derivative, total derivative, etc.

Refer to [5], let the value of a property per unit mass be denoted by ϕ . The total or substantive derivative of with respect to time following a fluid particle, written as $\frac{D\phi}{Dt}$, is

$$\frac{D\phi}{Dt} = \frac{\partial\phi}{\partial t} + \frac{\partial\phi}{\partial x} \frac{dx}{dt} + \frac{\partial\phi}{\partial y} \frac{dy}{dt} + \frac{\partial\phi}{\partial z} \frac{dz}{dt} \quad (1.4)$$

A fluid particle follows the flow, so $dx/dt = u$, $dy/dt = v$ and $dz/dt = w$. Hence the substantive derivative of ϕ is given by

$$\frac{D\phi}{Dt} = \frac{\partial\phi}{\partial t} + u \frac{\partial\phi}{\partial x} + v \frac{\partial\phi}{\partial y} + w \frac{\partial\phi}{\partial z} \quad (1.5)$$

$$= \frac{\partial\phi}{\partial t} + \mathbf{u} \cdot \nabla \phi \quad (1.6)$$

The derivative $\frac{D\phi}{Dt}$ defines rate of change of property ϕ per unit mass.

Definition 1.2.1 – Material derivative. The material derivative is defined for any tensor field ϕ that is macroscopic, with the sense that it depends only on position and time coordinates, $\phi = \phi(\mathbf{r}, t)$:

$$\frac{D\phi}{Dt} \equiv \frac{\partial\phi}{\partial t} + \mathbf{u} \cdot \nabla \phi \quad (1.7)$$

For a macroscopic vector field $\Phi(\mathbf{r}, t)$ the definition becomes

$$\frac{D\Phi}{Dt} \equiv \frac{\partial\Phi}{\partial t} + \mathbf{u} \cdot \nabla \Phi \quad (1.8)$$

The mass conservation equation contains the mass per unit volume (i.e. the density ρ) as the conserved quantity. The sum of the rate of change of density in time and the convective term in the mass conservation equation for a fluid element is

$$\boxed{\frac{\partial\rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0} \quad (1.9)$$

or in index notation:

$$\boxed{\partial_t \rho + \partial_\alpha (\rho u_\alpha) = 0} \quad (1.10)$$

Performing the chain differentiation of the second term in the mass conservation equation namely

$$\nabla \cdot (\rho \mathbf{u}) = \rho \nabla \cdot \mathbf{u} + \mathbf{u} \cdot \nabla \rho \quad (1.11)$$

or in index notation:

$$\partial_\alpha (\rho u_\alpha) = \rho (\partial_\alpha u_\alpha) + u_\alpha (\partial_\alpha \rho) \quad (1.12)$$

Thus the mass conservation equation becomes

$$\underbrace{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u})}_{\text{conservation form}} = \left(\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho \right) + \rho \nabla \cdot \mathbf{u} = \underbrace{\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u}}_{\text{non-conservation form}} = 0 \quad (1.13)$$

For incompressible flow, the condition for a working medium to be considered as incompressible is that the substantial change of its density along the flow path vanishes. This means that:

$$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho = 0 \quad (1.14)$$

or in index notation:

$$D_t \rho = \partial_t \rho + u_\alpha (\partial_\alpha \rho) \quad (1.15)$$

Thus, the continuity equation for an incompressible flow reduces to:

$$\nabla \cdot \mathbf{u} = 0 \quad (1.16)$$

or in index notation:

$$\partial_\alpha u_\alpha = 0 \quad (1.17)$$

or in longhand notation in a Cartesian coordinate system

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad (1.18)$$

From [5], for an arbitrary conserved property with a generalization form can be expresses the rate of change in time of ϕ per unit volume plus the net flow of ϕ out of the fluid element per unit volume. Then we rewritten to illustrate its relationship with the substantive derivative of ϕ :

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot (\rho\phi\mathbf{u}) = \rho \left(\frac{\partial\phi}{\partial t} + \mathbf{u} \cdot \nabla \phi \right) + \phi \left(\frac{\partial\rho}{\partial t} + \nabla \cdot (\rho\mathbf{u}) \right) \quad (1.19)$$

$$= \rho \frac{D\phi}{Dt} \quad (1.20)$$

This is because if we look $\rho\mathbf{u}$ as a whole,

$$\nabla \cdot (\rho\phi\mathbf{u}) = \phi \nabla \cdot (\rho\mathbf{u}) + \rho\mathbf{u} \cdot \nabla \phi \quad (1.21)$$

The term $\phi\{\partial\rho/\partial t + \nabla\cdot(\rho\mathbf{u})\}$ is equal to zero by virtue of mass conservation.

To construct the three components of the momentum equation and the energy equation the relevant entries for ϕ and their rates of change per unit volume are given below:

Table 1.2: Enter table caption here.

term	variable	non-conservative form	conservative form
x -momentum	u	$\rho(Du/\partial t)$	$\partial(\rho u)/\partial t + \nabla\cdot(\rho u\mathbf{u})$
y -momentum	v	$\rho(Dv/\partial t)$	$\partial(\rho v)/\partial t + \nabla\cdot(\rho v\mathbf{u})$
z -momentum	w	$\rho(Dw/\partial t)$	$\partial(\rho w)/\partial t + \nabla\cdot(\rho w\mathbf{u})$
energy	e	$\rho(De/\partial t)$	$\partial(\rho e)/\partial t + \nabla\cdot(\rho e\mathbf{u})$

The above process can be summarized in index notation, as

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) = \underbrace{\rho\left(\frac{\partial\mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right)}_{\text{material derivative}} + \underbrace{\mathbf{u}\left(\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u})\right)}_{\text{continuity equation}} \rightarrow 0 \quad (1.22)$$

$$= \rho \frac{D\mathbf{u}}{Dt} \quad (1.23)$$

Note that for the tensor product of the velocity vector $\mathbf{u}\otimes\mathbf{u}$ should follow (the tensor product of two vectors produces a second rank tensor):

$$\mathbf{u}\otimes\mathbf{u} = \mathbf{u}\mathbf{u}^T = \begin{bmatrix} u_\alpha \\ u_\beta \end{bmatrix} \begin{bmatrix} u_\alpha & u_\beta \end{bmatrix} = \begin{bmatrix} u_\alpha u_\alpha & u_\alpha u_\beta \\ u_\beta u_\alpha & u_\beta u_\beta \end{bmatrix} \quad (1.24)$$

If we have a bases for the vector spaces, and the vector spaces are finite-dimensional, we can represent the vectors in terms of components under those basis vectors:

$$\mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_m \end{bmatrix} \quad (1.25)$$

where each notation stands for the sum $\mathbf{v} = v_1\mathbf{e}_1 + v_2\mathbf{e}_2 + \cdots + v_n\mathbf{e}_n$

Given two vectors, we can form a tensor of their own from them rather naturally using the outer product, which is denoted $\mathbf{v}\otimes\mathbf{w}$ and equals $\mathbf{v}\mathbf{w}^T$. This tensor comes out as the matrix [3]:

$$\mathbf{v}\otimes\mathbf{w} = \begin{bmatrix} v_1 w_1 & v_1 w_2 & \cdots & v_1 w_m \\ v_2 w_1 & v_2 w_2 & \cdots & v_2 w_m \\ \vdots & \vdots & \ddots & \vdots \\ v_n w_1 & v_n w_2 & \cdots & v_n w_m \end{bmatrix} \quad (1.26)$$

1.2.1.3 Momentum Equation in Three Dimensions

Here introduce the derivation process of momentum equation ...

1.2.1.4 Energy Equation in Three Dimensions

Here introduce the derivation process of energy equation ...

1.2.2 Navier-Stokes Equations for Newtonian Fluid

The momentum equation for compressible Newtonian fluid will be:

$$\underbrace{\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u})}_{\text{conservation form}} = \underbrace{\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right)}_{\text{non-conservation form}} = \rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g} \quad (1.27)$$

where \mathbf{g} relates to body forces, such as gravitational, electromagnetic, etc.

For a Newtonian fluid viscous stress is proportional to velocity gradients:

$$\boldsymbol{\tau} = \mu \left\{ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right\} + \lambda (\nabla \cdot \mathbf{u}) \mathbf{I} = 2\mu \mathcal{D}(\mathbf{u}) + \lambda (\nabla \cdot \mathbf{u}) \mathbf{I} \quad (1.28)$$

where $\mathcal{D}(\mathbf{u}) = \frac{1}{2} \left\{ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right\}$ is the deformation tensor, μ is a (fluid-dependent) constant, referred to as viscosity, and $\lambda \approx -\frac{2}{3}\mu$.

Refer to [6], A straightforward substitution of $\boldsymbol{\tau}$ into the momentum conservation equation will yield the momentum part of the **Navier-Stokes equations**, describing the compressible Newtonian fluid:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot \left\{ \mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right\} + \nabla \cdot \left\{ \lambda (\nabla \cdot \mathbf{u}) \mathbf{I} \right\} + \rho \mathbf{g} \quad (1.29)$$

Often it is useful to rearrange the viscous stress terms as follows:

$$\begin{aligned} \nabla \cdot \left\{ \mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) + \lambda (\nabla \cdot \mathbf{u}) \mathbf{I} \right\} &= (\partial_x, \partial_y, \partial_z) \cdot \left\{ \mu (\partial_\beta u_\alpha + \partial_\alpha u_\beta) + \delta_{\alpha\beta} \lambda \partial_\gamma u_\gamma \right\} \\ &= \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \cdot \left\{ \mu \begin{bmatrix} 2\frac{\partial u}{\partial x} & \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \\ \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) & 2\frac{\partial v}{\partial y} & \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \\ \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) & \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right) & 2\frac{\partial w}{\partial z} \end{bmatrix} \right\} + \\ &\quad \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \cdot \left\{ \lambda \begin{bmatrix} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) & 0 & 0 \\ 0 & \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) & 0 \\ 0 & 0 & \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \end{bmatrix} \right\} \end{aligned} \quad (1.30)$$

Refer to [5], take the viscous terms of the x momentum equation as an example:

$$\begin{aligned}
& \frac{\partial}{\partial x} \left\{ 2\mu \frac{\partial u}{\partial x} + \lambda(\nabla \cdot \mathbf{u}) \right\} + \frac{\partial}{\partial y} \left\{ \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right\} + \frac{\partial}{\partial z} \left\{ \mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right\} \\
&= \frac{\partial}{\partial x} \left(\mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu \frac{\partial u}{\partial z} \right) \\
&\quad + \left\{ \frac{\partial}{\partial x} \left(\mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial z} \left(\mu \frac{\partial w}{\partial x} \right) + \frac{\partial}{\partial x} (\lambda \nabla \cdot \mathbf{u}) \right\} \\
&= \nabla \cdot (\mu \nabla u) + [S_{Mx}]
\end{aligned} \tag{1.31}$$

The viscous stresses in the y - and z -component equations can be recast in a similar manner. We simplify the viscous stress equations by “hiding” the smaller contributions of the viscous stress terms into a bracketed $[S_{Mx}]$ as a momentum source.

For Newtonian fluid, the viscosity μ remains constant, no matter the amount of shear applied for a constant temperature. These fluids have a linear relationship between viscosity and shear stress.

Thus, for $\lambda = -\frac{2}{3}\mu$, the viscous terms of the x momentum equation will be:

$$\begin{aligned}
& \frac{\partial}{\partial x} \left\{ 2\mu \frac{\partial u}{\partial x} + \lambda(\nabla \cdot \mathbf{u}) \right\} + \frac{\partial}{\partial y} \left\{ \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right\} + \frac{\partial}{\partial z} \left\{ \mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right\} \\
&= \frac{\partial}{\partial x} \left(\mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu \frac{\partial u}{\partial z} \right) \\
&\quad + \left\{ \frac{\partial}{\partial x} \left(\mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial z} \left(\mu \frac{\partial w}{\partial x} \right) + \frac{\partial}{\partial x} (\lambda \nabla \cdot \mathbf{u}) \right\} \\
&= \left(\mu \frac{\partial^2 u}{\partial x^2} + \mu \frac{\partial^2 u}{\partial y^2} + \mu \frac{\partial^2 u}{\partial z^2} \right) + \mu \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) + \lambda \frac{\partial}{\partial x} (\nabla \cdot \mathbf{u}) \\
&= \boxed{\mu \nabla^2 u + (\mu + \lambda) \frac{\partial}{\partial x} (\nabla \cdot \mathbf{u})}
\end{aligned} \tag{1.32}$$

$$= \mu \Delta u + \frac{\mu}{3} \frac{\partial}{\partial x} (\nabla \cdot \mathbf{u}) \tag{1.33}$$

same process can be derived for the viscous terms of the y and z momentum equations.

We can also use the relation $\nabla \cdot (\nabla \mathbf{u})^T = \nabla(\nabla \cdot \mathbf{u})$, thus

$$\boxed{\nabla \cdot (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) = \nabla^2 \mathbf{u} + \nabla \cdot (\nabla \mathbf{u})^T = \nabla^2 \mathbf{u} + \nabla(\nabla \cdot \mathbf{u})} \tag{1.34}$$

Also, seems that the following equation is correct for the **identity matrix I**:

$$\nabla \cdot \{ \lambda(\nabla \cdot \mathbf{u}) \mathbf{I} \} = \lambda \nabla(\nabla \cdot \mathbf{u}) \tag{1.35}$$

Thus, the divergence of the viscous stress term $\nabla \cdot \boldsymbol{\tau}$ will be:

$$\begin{aligned}
\nabla \cdot \boldsymbol{\tau} &= \nabla \cdot \left\{ \mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right\} + \nabla \cdot \{ \lambda (\nabla \cdot \mathbf{u}) \mathbf{I} \} \\
&= \mu \nabla^2 \mathbf{u} + \mu \nabla (\nabla \cdot \mathbf{u}) + \lambda \nabla (\nabla \cdot \mathbf{u}) \\
&= \boxed{\mu \nabla^2 \mathbf{u} + (\mu + \lambda) \nabla (\nabla \cdot \mathbf{u})} \\
&= \mu \Delta \mathbf{u} + \frac{\mu}{3} \nabla (\nabla \cdot \mathbf{u})
\end{aligned}$$

We can update the the **Navier-Stokes equations** in Eq. (1.29) as

$$\begin{cases} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \\ \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \Delta \mathbf{u} + \frac{\mu}{3} \nabla (\nabla \cdot \mathbf{u}) + \rho \mathbf{g} \end{cases} \quad (1.36)$$

in which, the Laplace operator Δ is a second order differential operator in the n -dimensional Euclidean space, defined as the divergence ($\nabla \cdot$) of the gradient (∇g), i.e. $\Delta g = \nabla \cdot \nabla g = \nabla^2 g$.

For the special (but very common) case of incompressible flow, the viscosity μ will now be a constant, and the second viscosity effect $\lambda (\nabla \cdot \mathbf{u}) \mathbf{I}$ in the viscous stress tensor $\boldsymbol{\tau}$ will vanish. Along with the vanish is the $\mu \nabla (\nabla \cdot \mathbf{u})$ term. So the total $\frac{\mu}{3} \nabla (\nabla \cdot \mathbf{u})$ term will vanish, refer to the compressible Navier Stokes equations in (1.36). This gives **incompressible Navier Stokes equations**, describing incompressible Newtonian fluid:

$$\begin{aligned}
\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) &= -\nabla p + \nabla \cdot \left\{ \mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right\} + \nabla \cdot \{ \lambda (\nabla \cdot \mathbf{u}) \mathbf{I} \} + \rho \mathbf{g} \\
&= -\nabla p + \mu \Delta \mathbf{u} + \rho \mathbf{g}
\end{aligned}$$

This indicates that the first viscosity effect $\mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right)$ in the viscous stress tensor $\boldsymbol{\tau}$ can be simplified by using the continuity equation $\nabla \cdot \mathbf{u} = 0$ for incompressible flow. We consider the viscous terms of the x momentum equation again:

$$\begin{aligned}
&\frac{\partial}{\partial x} \left(2\mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left\{ \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right\} + \frac{\partial}{\partial z} \left\{ \mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right\} \\
&= 2\mu \frac{\partial^2 u}{\partial x^2} + \mu \frac{\partial^2 v}{\partial y \partial x} + \mu \frac{\partial^2 u}{\partial y^2} + \mu \frac{\partial^2 w}{\partial z \partial x} + \mu \frac{\partial^2 u}{\partial z^2} \\
&= \left(\mu \frac{\partial^2 u}{\partial x^2} + \mu \frac{\partial^2 u}{\partial y^2} + \mu \frac{\partial^2 u}{\partial z^2} \right) + \left(\mu \frac{\partial^2 v}{\partial y \partial x} + \mu \frac{\partial^2 w}{\partial z \partial x} \right) \\
&= \mu \nabla^2 u + \mu \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \xrightarrow{0} \\
&= \mu \nabla^2 u
\end{aligned} \quad (1.37)$$

Similarly for the y and z momentum directions we have $\mu \nabla^2 v$ and $\mu \nabla^2 w$.

Then the momentum conservation equation for incompressible flow will be simplified, as

$$\boxed{\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \Delta \mathbf{u} + \mathbf{g}} \quad (1.38)$$

Again, the Laplace operator $\Delta = \nabla \cdot \nabla = \nabla^2$.

In Cartesian index notation, we have:

$$\partial_t u_\alpha + u_\beta (\partial_\beta u_\alpha) = -\frac{1}{\rho} \partial_\alpha p + \nu \partial_\beta (\partial_\beta u_\alpha) + g_\alpha \quad (1.39)$$

Using the Einstein summation convention, the three components are:

$$\begin{cases} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + g_x \\ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) + g_y \\ \frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} + \nu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) + g_z \end{cases} \quad (1.40)$$

Finally, the **incompressible Navier Stokes equations** for incompressible Newtonian fluid are:

$$\boxed{\begin{cases} \nabla \cdot \mathbf{u} = 0 \\ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{g} \end{cases}} \quad (1.41)$$

in which $\nu = \mu/\rho$ is the kinematic viscosity of the fluid (m²/sec). Or in index notation:

$$\boxed{\begin{cases} \partial_\alpha u_\alpha = 0 \\ \partial_t u_\alpha + u_\beta (\partial_\beta u_\alpha) = -\frac{1}{\rho} \partial_\alpha p + \nu \partial_\beta (\partial_\beta u_\alpha) + g_\alpha \end{cases}} \quad (1.42)$$

1.2.3 Equations of State

The motion of a fluid in three dimensions is described by a system of five partial differential equations: mass conservation (1.9), x , y and z momentum equations (1.29) and **energy equation**. There are totally seven unknown variables: the velocities u , v , w , the density ρ , the pressure p , the internal energy e and the temperature T . Among the unknowns are four thermodynamic variables: the density ρ , the pressure p , the internal energy e and the temperature T . In this brief discussion we point out the linkage between these four variables. Relationships between the thermodynamic variables can be obtained through the assumption of thermodynamic equilibrium. The fluid velocities may be large, but they are usually small enough that, even though properties of a fluid particle change rapidly from place to place, the fluid can thermodynamically adjust itself to new conditions so quickly that the changes are effectively instantaneous. Thus the fluid always remains in thermodynamic equilibrium. The only exceptions are certain flows with strong shock waves, but even some of those are often well enough approximated by equilibrium assumptions [5].

We can describe the state of a substance in thermodynamic equilibrium by means of just two state variables. Equations of state relate the other variables to the two state variables. If we use ρ and T as state variables we have state equations for pressure p and specific internal energy e :

$$p = p(\rho, T) \quad \text{and} \quad e = e(\rho, T) \quad (1.43)$$

For a perfect gas the following, well-known, equations of state are useful [5]:

$$P = \rho R_{\text{specific}} T \quad \text{and} \quad e = C_V T \quad (1.44)$$

The relations will be introduced in Eq. (1.78) and Eq. (1.91).

The assumption of thermodynamic equilibrium eliminates all but the two thermodynamic state variables. In the flow of compressible fluids the equations of state provide the linkage between the energy equation on the one hand and mass conservation and momentum equations on the other. This linkage arises through the possibility of density variations as a result of pressure and temperature variations in the flow field.

Liquids and gases flowing at low speeds behave as incompressible fluids. Without density variations there is no linkage between the energy equation and the mass conservation and momentum equations. The flow field can often be solved by considering mass conservation and momentum equations only. The energy equation only needs to be solved alongside the others if the problem involves heat transfer.

1.3 Kinetic Theory

1.3.1 Maxwell-Boltzmann Distribution

Temperature of a gas is a measure of the kinetic energy of the particles. Even at a constant temperature, however, not all the molecules have the same speed. After all, in a gas there are permanent collisions between the particles. Some particles are slowed down by the collision and others are accelerated by it. Thus, molecules with different velocities can be found.

A gas usually contains a large number of molecules. For ideal gases, therefore, statistical predictions can be made about the frequency with which certain speeds occur. The Maxwell-Boltzmann distribution describes the speed distribution of the particles of an ideal gas. [7]

In physics (in particular in statistical mechanics), the Maxwell-Boltzmann distribution is a particular probability distribution named after James Clerk Maxwell and Ludwig Boltzmann [8].

It was first defined and used for describing particle speeds in idealized gases, where the particles move freely inside a stationary container without interacting with one another, except for very brief collisions in which they exchange energy and momentum with each other or with their thermal environment. The term “particle” in this context refers to gaseous particles only (atoms or molecules), and the system of particles is assumed to have reached thermodynamic equilibrium. The energies of such particles follow what is known as Maxwell-Boltzmann statistics, and the statistical distribution of speeds is derived by equating particle energies with kinetic energy [8]. The Maxwell-Boltzmann distribution function of the molecular speed of ideal gases can be derived from the barometric formula. This article shows the derivation [9].

The Maxwell-Boltzmann distribution is a result of the kinetic theory of gases, which provides a simplified explanation of many fundamental gaseous properties, including pressure and diffusion. The Maxwell-Boltzmann distribution applies fundamentally to particle velocities in three dimensions, but turns out to depend only on the speed (the magnitude of the velocity) of the particles. A particle speed probability distribution indicates which speeds are more likely: a particle will have a speed selected randomly from the distribution, and is more likely to be within one range of speeds than another.

Assuming the system of interest contains a large number of particles, the fraction of the parti-

cles within an infinitesimal element of three-dimensional velocity space (in a Cartesian coordinate system), $dv_x dv_y dv_z$, centered on a velocity vector of magnitude v is $f_{\mathbf{v}}(v) dv_x dv_y dv_z$ (the probability of finding a particle with velocity in the infinitesimal element $[dv_x, dv_y, dv_z]$ about velocity $\mathbf{v} = [v_x, v_y, v_z]$ and squared velocity magnitude $v^2 = v_x^2 + v_y^2 + v_z^2$), in which

$$f_{\mathbf{v}}(v) dv_x dv_y dv_z = \left(\frac{m}{2\pi kT} \right)^{3/2} \exp\left(-\frac{mv^2}{2kT} \right) dv_x dv_y dv_z \quad (1.45)$$

Thus we obtain the Maxwell's distribution for the velocity vector:

$$f_{\mathbf{v}}(v) = \left(\frac{m}{2\pi kT} \right)^{3/2} \exp\left(-\frac{mv^2}{2kT} \right) \quad (1.46)$$

where m is the particle mass (mass of a particle, not the total mass of the gas!), the constant k is the so-called Boltzmann constant with a value of $k = 1.38065 \times 10^{-23} \frac{\text{m}^2 \cdot \text{kg}}{\text{s}^2 \cdot \text{K}}$ in SI base units [10], and the temperature T must be expressed in the unit Kelvin. The distribution of the molecular speeds for an ideal gas is independent of the gas pressure.

The Maxwell distribution for particles moving in only one direction, for example x , is given by:

$$f_{\mathbf{v}}(v_x) = \left(\frac{m}{2\pi kT} \right)^{1/2} \exp\left(-\frac{mv_x^2}{2kT} \right) \quad (1.47)$$

Here $f_{\mathbf{v}}(v)$ is given as a probability distribution function, properly normalized so that integration of $f_{\mathbf{v}}(v)$ over all velocities equals one:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_{\mathbf{v}}(v) dv_x dv_y dv_z = \int_{-\infty}^{\infty} f_{\mathbf{v}}(v_x) dv_x = \int_{-\infty}^{\infty} f_{\mathbf{v}}(v_y) dv_y = \int_{-\infty}^{\infty} f_{\mathbf{v}}(v_z) dv_z = 1 \quad (1.48)$$

In D -dimensional space, the Maxwell distribution becomes:

$$f_{\mathbf{v}}(v) = \left(\frac{m}{2\pi kT} \right)^{D/2} \exp\left(-\frac{mv^2}{2kT} \right) \quad (1.49)$$

Note that the probability distribution is often multiplied by the particle density, so that the integral of the resulting distribution function equals the density.

However, the equation above is redundant and not concise, because the symmetry of $f(v)$ is not considered. Because we can clearly see that $f(v)$ is really not relates to the individual velocity components (v_x, v_y, v_z) , rather the velocity magnitude $v^2 = v_x^2 + v_y^2 + v_z^2$ matters. This means that for ideal gas, the velocity direction is not important and we need to sum over all directions. One way to visualize that sum is as the development of a spherical shell volume element in “velocity space”.

Consider the symmetries of the integrands. If an integrand is spherically symmetric about $\mathbf{v} = 0$, the substitution $d\mathbf{v} = dv_x dv_y dv_z = 4\pi v^2 dv = 4\pi |\mathbf{v}|^2 d|\mathbf{v}|$

We introduce in the velocity space (v_x, v_y, v_z) spherical coordinates (v, θ, ϕ) as indicated in Fig. 1.1 (note that illustration here is regular space not velocity space). Then the volume element in velocity space is given by $dv_x dv_y dv_z = v^2 dv \sin\theta d\theta d\phi = v^2 dv d\Omega$ in the spherical coordinate system, where ϕ and θ are the spherical coordinate angles of the velocity vector \mathbf{v} . Integration of

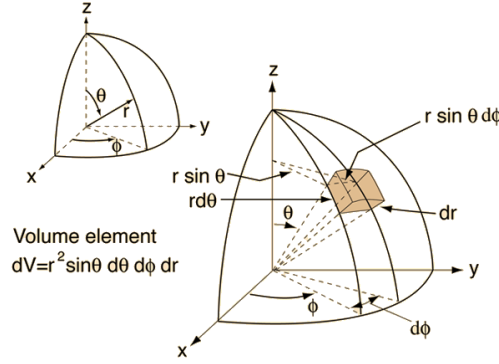


Figure 1.1: Spherical Polar Coordinates

the probability density function of the velocity over the solid angles $d\Omega$ yields an additional factor of 4π , i.e. $\int d\Omega = \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi = 4\pi$, or $dv_x dv_y dv_z = 4\pi v^2 dv$.

Thus, the probability that a molecule has speed between $(v, v + dv)$ with a direction expressed with $\{(\theta, \theta + d\theta), (\phi, \phi + d\phi)\}$ is:

$$f_{\mathbf{v}}(v) dv_x dv_y dv_z = f_{\mathbf{v}}(v) v^2 dv \sin\theta d\theta d\phi \quad (1.50)$$

Considering the symmetry of $f_{\mathbf{v}}(v)$ in velocity direction, we transform the integration coordinates and sum over all directions:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_{\mathbf{v}}(v) dv_x dv_y dv_z = \int_0^{\infty} \int_0^\pi \int_0^{2\pi} f_{\mathbf{v}}(v) v^2 dv \sin\theta d\theta d\phi = 4\pi \int_0^{\infty} f_{\mathbf{v}}(v) v^2 dv \quad (1.51)$$

The speed distribution with substitution of the speed for the sum of the squares of the vector components:

$$f(v) = \left(\frac{m}{2\pi kT}\right)^{3/2} (4\pi v^2) \exp\left(-\frac{mv^2}{2kT}\right) = \left(\frac{2}{\pi}\right)^{1/2} \left(\frac{m}{kT}\right)^{3/2} v^2 \exp\left(-\frac{mv^2}{2kT}\right) \quad (1.52)$$

It's obvious that $f(v)$ is equivalent to $f_{\mathbf{v}}(v)$, but $f(v)$ is more concise, and takes advantage the symmetry of the velocity space. We will consider the integration of the distribution function.

1.3.2 Evaluation of Gaussian Integrals

We need to evaluate integrals of the form:

$$I_n = \int_0^{\infty} x^n e^{-ax^2} dx \quad (1.53)$$

We can tackle this first by integrating by parts:

Theorem 1.3.1 – Integration by parts. In calculus, and more generally in mathematical analysis, integration by parts or partial integration is a process that finds the integral of a product of functions in terms of the integral of the product of their derivative and antiderivative. The rule can be thought of as an integral version of the product rule of differentiation.

If $u = u(x)$ and $du = u'(x)dx$, while $v = v(x)$ and $dv = v'(x)dx$, the product rule of differentiation states that:

$$\frac{d}{dx}(uv) = u \frac{dv}{dx} + v \frac{du}{dx} \quad (1.54)$$

Rearranging, we have:

$$u \frac{dv}{dx} = \frac{d}{dx}(uv) - v \frac{du}{dx} \quad (1.55)$$

Integrating throughout with respect to dx on both sides, we obtain the formula for integration by parts:

$$\int u \frac{dv}{dx} dx = uv - \int v \frac{du}{dx} dx \quad (1.56)$$

or more compactly:

$$\int u dv = uv - \int v du \quad (1.57)$$

For definite integral, the integration by parts states that:

$$\begin{aligned} \int_a^b u(x)v'(x)dx &= [u(x)v(x)]_a^b - \int_a^b u'(x)v(x)dx \\ &= u(b)v(b) - u(a)v(a) - \int_a^b u'(x)v(x)dx \end{aligned} \quad (1.58)$$

$$\begin{aligned} I_n &= -\frac{1}{2a} \int_0^\infty x^{n-1}(-2ax)e^{-ax^2} dx \\ &= -\frac{1}{2a} \left[x^{n-1}e^{-ax^2} \right]_0^\infty + \frac{1}{2a} \int_0^\infty (n-1)x^{n-2}e^{-ax^2} dx \\ &= \frac{n-1}{2a} I_{n-2} \end{aligned}$$

This is known as a reduction formula, and using it we can (eventually) evaluate any integral I_n we need if we know I_0 and I_1 .

The value of $\frac{1}{2a} \left[x^{n-1}e^{-ax^2} \right]_0^\infty$ equals 0 for both ends, this is because of the L'Hospital's rule in Theorem 1.3.2. In mathematics, more specifically calculus, L'Hospital's rule provides a technique to evaluate limits of indeterminate forms.

Theorem 1.3.2 – L'Hospital's rule for zero over zero. Suppose that $\lim_{x \rightarrow a} f(x) = 0$, $\lim_{x \rightarrow a} g(x) = 0$, and that functions f and g are differentiable on an open interval I except possibly at a point a contained in I . Assume also that $g'(x) \neq 0$ for all x in I if $x \neq a$. Then

$$\lim_{x \rightarrow a} \frac{f(x)}{g(x)} = \lim_{x \rightarrow a} \frac{f'(x)}{g'(x)} \quad (1.59)$$

Similar results hold for $x \rightarrow \infty$ and $x \rightarrow -\infty$.

Theorem 1.3.3 – L'Hospital's rule for infinity over infinity. Assume that functions f and g are

differentiable for all x larger than some fixed number. If $\lim_{x \rightarrow a} f(x) = \infty$ and $\lim_{x \rightarrow a} g(x) = \infty$, then

$$\lim_{x \rightarrow a} \frac{f(x)}{g(x)} = \lim_{x \rightarrow a} \frac{f'(x)}{g'(x)} \quad (1.60)$$

Similar results hold for $x \rightarrow \infty$ and $x \rightarrow -\infty$.

Then we can calculate the limit of $\lim_{x \rightarrow \infty} \frac{x^{n-1}}{e^{ax^2}}$. The function has an indeterminate form of type $\frac{\infty}{\infty}$. Let $y = x^2$ and $x \rightarrow \infty \Rightarrow y \rightarrow \infty$. Apply L'Hopital's rule $(n-1)$ times:

$$\begin{aligned} \lim_{x \rightarrow \infty} \frac{x^{n-1}}{e^{ax^2}} &= \lim_{y \rightarrow \infty} \frac{y^{(n-1)/2}}{e^{ay}} \\ &= \begin{cases} \lim_{y \rightarrow \infty} \frac{\frac{(n-1)!}{2}}{a^{(n-1)/2} e^{ay}} = 0, & \text{if } n > 1 \text{ and } (n-1) \text{ is an even number} \\ \lim_{y \rightarrow \infty} \frac{\frac{n!}{2}}{a^{n/2} y^{1/2} e^{ay}} = 0, & \text{if } n > 1 \text{ and } (n-1) \text{ is an odd number} \end{cases} \end{aligned}$$

If $n = 1$, the result is obvious to be zero. Thus we can prove $\frac{1}{2a} [x^{n-1} e^{-ax^2}]_0^\infty = 0$.

I_1 can be integrated directly:

$$\begin{aligned} I_1 &= \int_0^\infty x e^{-ax^2} dx \\ &= -\frac{1}{2a} \int_0^\infty (1)(-2ax) e^{-ax^2} dx \\ &= -\frac{1}{2a} [e^{-ax^2}]_0^\infty \\ &= \frac{1}{2a} \end{aligned}$$

I_0 is a little more tricky (this is the usual Gaussian integral). To evaluate it, first consider the square of the integral, written as

$$\begin{aligned} I_0^2 &= \int_0^\infty e^{-ax^2} dx \int_0^\infty e^{-ay^2} dy \\ &= \int_0^\infty \int_0^\infty e^{-a(x^2+y^2)} dx dy \end{aligned}$$

This is the volume under a two-dimensional gaussian curve, over the positive quarter of the (x, y) plane. In polar coordinates we can write this same volume in terms of r , where $r^2 = x^2 + y^2$, as

$$\begin{aligned}
I_0^2 &= \int_0^\infty \int_0^{\frac{\pi}{2}} e^{-ar^2} r dr d\theta \\
&= -\frac{\pi}{4a} \int_0^\infty (-2ar) e^{-ar^2} dr \\
&= -\frac{\pi}{4a} \left[e^{-ar^2} \right]_0^\infty \\
&= \frac{\pi}{4a}
\end{aligned}$$

So we obtain $I_0 = \int_0^\infty e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}$. (Note that $\int_{-\infty}^\infty e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$, a comprehensive description of how this is done in [11])

So finally, we can present the full reduction formula:

If

$$I_n = \int_0^\infty x^n e^{-ax^2} dx \quad (1.61)$$

then

$$I_0 = \frac{1}{2} \sqrt{\frac{\pi}{a}} \quad (1.62a)$$

$$I_1 = \frac{1}{2a} \quad (1.62b)$$

$$I_n = \frac{n-1}{2a} I_{n-2} \quad (1.62c)$$

One can now evaluate in particular the following integrals [11, 12]:

$$I_0(a) = \int_0^\infty e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}} \quad (1.63a)$$

$$I_1(a) = \int_0^\infty x e^{-ax^2} dx = \frac{1}{2a} \quad (1.63b)$$

$$I_2(a) = \int_0^\infty x^2 e^{-ax^2} dx = \frac{1}{4a} \sqrt{\frac{\pi}{a}} \quad (1.63c)$$

$$I_3(a) = \int_0^\infty x^3 e^{-ax^2} dx = \frac{1}{2a^2} \quad (1.63d)$$

$$I_4(a) = \int_0^\infty x^4 e^{-ax^2} dx = \frac{3}{8a^2} \sqrt{\frac{\pi}{a}} \quad (1.63e)$$

$$I_5(a) = \int_0^\infty x^5 e^{-ax^2} dx = \frac{1}{a^3} \quad (1.63f)$$

$$I_6(a) = \int_0^\infty x^6 e^{-ax^2} dx = \frac{15}{16a^3} \sqrt{\frac{\pi}{a}} \quad (1.63g)$$

$$I_7(a) = \int_0^\infty x^7 e^{-ax^2} dx = \frac{3}{a^4} \quad (1.63h)$$

Actually the solution can be summarized as follows (refer the discussion of the Gamma Function by Weber and Arfken [13]):

$$I_n = \int_0^\infty x^n e^{-ax^2} dx = \begin{cases} \frac{(n-1)!!}{2^{\frac{n}{2}+1} a^{\frac{n}{2}}} \sqrt{\frac{\pi}{a}} & \text{for } n \text{ even} \\ \frac{\{\frac{1}{2}(n-1)\}!}{2a^{\frac{(n+1)}{2}}} & \text{for } n \text{ odd} \end{cases} \quad (1.64)$$

In mathematics, the double factorial of a positive integer n (denoted by $n!!$) is the product of all the integers from 1 up to n that have the same parity (odd or even) as n , that is,

$$n!! = \begin{cases} n \cdot (n-2) \cdot \dots \cdot 5 \cdot 3 \cdot 1 & n > 0 \text{ odd} \\ n \cdot (n-2) \cdot \dots \cdot 6 \cdot 4 \cdot 2 & n > 0 \text{ even} \\ 1 & n = -1, 0 \end{cases} \quad (1.65)$$

Note that $-1!! = 0!! = 1$ by definition. The factorial of a non-zero n may be written as the product of two double factorials: $n! = n!! \cdot (n-1)!!$.

The following integral will also be useful:

$$H_n = \int_{-\infty}^\infty x^n e^{-ax^2} dx = \begin{cases} 2I_n & \text{for } n \text{ even} \\ 0 & \text{for } n \text{ odd} \end{cases} \quad (1.66)$$

Now we can define the Gaussian integral [14].

Definition 1.3.1 – Gaussian integral. The Gaussian integral, also known as the Euler-Poisson integral, is the integral of the Gaussian function^a e^{-x^2} over the entire real line. The integral is:

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi} \quad (1.67)$$

The definite integral of an arbitrary Gaussian function is

$$\int_{-\infty}^{\infty} e^{-a(x+b)^2} dx = \int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \quad (1.68)$$

This means that the area under the distribution function along the axis will not change when the distribution function moves along the axis.

An alternative form is

$$\int_{-\infty}^{\infty} e^{-ax^2+bx+c} dx = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}+c} \quad (1.69)$$

where a must be strictly positive for the integral to converge. The result is obvious if we split the polynomial:

$$\begin{aligned} -ax^2 + bx + c &= -a\left(x^2 - \frac{b}{a}x\right) + c \\ &= -a\left(x^2 - 2\frac{b}{2a}x + \frac{b^2}{4a^2}\right) + \frac{b^2}{4a} + c \\ &= -a\left(x - \frac{b}{2a}\right)^2 + \frac{b^2}{4a} + c \end{aligned}$$

The integral of an **arbitrary Gaussian function** is

$$\int_{-\infty}^{\infty} ae^{-(x-b)^2/2c^2} dx = a\sqrt{2\pi c^2} \quad (1.70)$$

for arbitrary real constants a , b and non zero c .

^aIn mathematics, a Gaussian function, often simply referred to as a Gaussian, is a function of the form: $f(x) = ae^{-\frac{(x-b)^2}{2c^2}}$ for arbitrary real constants a , b and non zero c .

Note that $\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$, the variable of integration is changed from x to $x = y + b$, and we have $dx = dy$ since b is constant, so we can prove that $\int_{-\infty}^{\infty} e^{-a(y+b)^2} dy = \int_{-\infty}^{\infty} e^{-a(x+b)^2} dx = \sqrt{\frac{\pi}{a}}$. Following the same method we can prove the integral of an arbitrary Gaussian function.

Now we consider this form of Gaussian integral, $\int_{-\infty}^{\infty} xe^{-a(x+b)^2} dx$. We will also use a new integration variable $y = x + b$, with $dx = d(x + b) = dy$ since b is a constant. By considering $\int_{-\infty}^{\infty} xe^{-ax^2} dx = 0$ since the integrand is a odd function, and $\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$, we have

$$\begin{aligned}
\int_{-\infty}^{\infty} x e^{-a(x+b)^2} dx &= \int_{-\infty}^{\infty} (x+b) e^{-a(x+b)^2} d(x+b) - \int_{-\infty}^{\infty} b e^{-a(x+b)^2} d(x+b) \\
&= \int_{-\infty}^{\infty} y e^{-ay^2} dy - b \int_{-\infty}^{\infty} e^{-ay^2} dy \\
&= -b \int_{-\infty}^{\infty} e^{-ay^2} dy \\
&= -b \sqrt{\frac{\pi}{a}}
\end{aligned}$$

Now we consider another form of Gaussian integral, $\int_{-\infty}^{\infty} x^2 e^{-a(x+b)^2} dx$. We still use a new integration variable $y = x + b$, with $dx = d(x+b) = dy$ since b is a constant. By considering $\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{1}{2a} \sqrt{\frac{\pi}{a}}$, $\int_{-\infty}^{\infty} x e^{-a(x+b)^2} dx = -b \sqrt{\frac{\pi}{a}}$, and $\int_{-\infty}^{\infty} e^{-a(x+b)^2} dx = \sqrt{\frac{\pi}{a}}$, we have

$$\begin{aligned}
\int_{-\infty}^{\infty} x^2 e^{-a(x+b)^2} dx &= \int_{-\infty}^{\infty} (x+b)^2 e^{-a(x+b)^2} dx - 2b \int_{-\infty}^{\infty} x e^{-a(x+b)^2} dx - b^2 \int_{-\infty}^{\infty} e^{-a(x+b)^2} dx \\
&= \int_{-\infty}^{\infty} y^2 e^{-ay^2} dy - 2b \left(-b \sqrt{\frac{\pi}{a}} \right) - b^2 \sqrt{\frac{\pi}{a}} \\
&= \frac{1}{2a} \sqrt{\frac{\pi}{a}} + b^2 \sqrt{\frac{\pi}{a}}
\end{aligned}$$

Now we can integrate the Maxwell's distribution for the velocity vector in x direction, by utilizing $H_0 = 2I_0 = \sqrt{\frac{\pi}{a}}$:

$$\begin{aligned}
\int_{-\infty}^{\infty} f_{\mathbf{v}}(v_x) dv_x &= \int_{-\infty}^{\infty} \left(\frac{m}{2\pi kT} \right)^{1/2} \exp\left(-\frac{mv_x^2}{2kT} \right) dv_x \\
&= \left(\frac{m}{2\pi kT} \right)^{1/2} \left(\frac{2k\pi T}{m} \right)^{1/2} = 1
\end{aligned}$$

Thus we obtain for all velocity components $\int_0^{\infty} \int_0^{\infty} \int_0^{\infty} f_{\mathbf{v}}(v) dv_x dv_y dv_z = 1$. Now we consider the integral of Maxwell's distribution for velocity magnitude $f(v)$, by utilizing $I_2 = \frac{1}{4a} \sqrt{\frac{\pi}{a}}$:

$$\begin{aligned}
\int_0^{\infty} f(v) dv &= \int_0^{\infty} \left(\frac{m}{2\pi kT} \right)^{3/2} (4\pi v^2) \exp\left(-\frac{mv^2}{2kT} \right) dv \\
&= \left(\frac{m}{2\pi kT} \right)^{3/2} (4\pi) \frac{1}{4} \left(\frac{2kT}{m} \right) \left(\frac{2k\pi T}{m} \right)^{1/2} = 1
\end{aligned}$$

Not that the integration interval of $f_{\mathbf{v}}(v_x)$ is $(-\infty, \infty)$ since v_x can be negative, while the integration of $f(v)$ is $(0, \infty)$ since the velocity magnitude v cannot be negative.

1.3.3 Typical Speeds

The mean speed $\langle v \rangle$, most probable speed (mode) v_p , and root-mean-square speed $v_{\text{rms}} = \sqrt{\langle v^2 \rangle}$ can be obtained from properties of the Maxwell distribution.

The most probable speed, v_p , is the speed most likely to be possessed by any molecule (of the same

mass m) in the system and corresponds to the maximum value or mode of $f(v)$. To find it, we calculate the derivative df/dv , set it to zero and solve for v :

$$\begin{aligned}\frac{df(v)}{dv} &= (4\pi) \left(\frac{m}{2\pi kT} \right)^{3/2} \left\{ (2v) \exp\left(-\frac{mv^2}{2kT}\right) + v^2 \left(-\frac{m}{2kT}\right) (2v) \exp\left(-\frac{mv^2}{2kT}\right) \right\} \\ &= -(8\pi v) \left(\frac{m}{2\pi kT} \right)^{3/2} \exp\left(-\frac{mv^2}{2kT}\right) \left\{ \left(\frac{mv^2}{2kT} \right) - 1 \right\}\end{aligned}$$

with the condition $\frac{mv_p^2}{2kT} = 1$, we get the solution of v_p :

$$\boxed{v_p = \sqrt{\frac{2kT}{m}} = \sqrt{\frac{2RT}{M}}} \quad (1.71)$$

in which, R is the gas constant and M is molar mass of the substance, and thus may be calculated as a product of particle mass m , and Avogadro constant N_A , as $M = mN_A$. Note if molar mass M is used, then the gas constant R should be used in the expression. If the mass m of an individual molecule is used instead, the expression would be the same except that Boltzmann constant k would be used instead of the molar gas constant R .

Definition 1.3.2 – Avogadro number. The Avogadro number, usually denoted by N_A , is the number of constituent particles (usually molecules, atoms or ions) that are contained in one mole, the international (SI) unit of amount of substance: by definition, exactly $6.02214076 \times 10^{23}$, and it is dimensionless. Specifically one mol is $6.02214076 \times 10^{23}$ molecules of a substance.

Definition 1.3.3 – Boltzmann constant. The Boltzmann constant k is a physical constant that relates the average relative kinetic energy of particles in a gas with the temperature of the gas (the average kinetic energy per molecule $\frac{1}{2}m\overline{v^2} = \frac{3}{2}kT$). The Boltzmann constant has the dimension of energy divided by temperature, the same as entropy. The Boltzmann constant is one of the seven “defining constants” that have been given exact definitions. The Boltzmann constant is defined to be exactly $1.380649 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$.

Definition 1.3.4 – Gas constant. The gas constant R is defined as the Avogadro constant N_A multiplied by the Boltzmann constant k : $R = N_A k$. As a consequence, the value of the gas constant is exactly $8.31446261815324 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$. Note that the numerical value of Avogadro constant is defined as being the Avogadro number, and its unit is the reciprocal of mole.

From the ideal gas law, which will be discussed later, $PV = nRT = NkT$, in which n is the amount of substance of gas (also known as number of moles), N is the number of gas molecules (or the Avogadro constant times the amount of substance $N = nN_A$). Thus we can also get the relation that $R = N_A k$.

Definition 1.3.5 – Molar mass. Since 2019, a mole of any substance has been redefined in the SI as the amount of that substance containing an exactly defined number of particles, $6.02214076 \times 10^{23}$ (Avogadro number). Therefore, the molar mass M of a compound now is simply the mass of this number of molecules of the compound.

We can get the following relation:

$$\frac{R}{M} = \frac{N_A k}{N_A m} = \frac{k}{m} \quad (1.72)$$

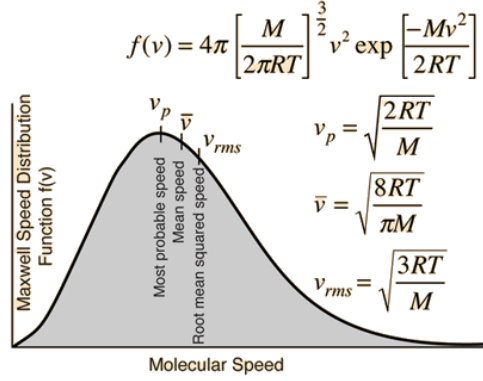


Figure 1.2: Maxwell Speed Distribution

The mean speed is the expected value of the speed distribution. From $I_3 = \int_0^\infty x^3 e^{-ax^2} dx = \frac{1}{2a^2}$ we can get (note that v is the velocity magnitude, with $v^2 = v_x^2 + v_y^2 + v_z^2$)

$$\begin{aligned}
 \langle v \rangle &= \int_0^\infty v f(v) dv \\
 &= \int_0^\infty \left(\frac{m}{2\pi kT} \right)^{3/2} (4\pi v^3) \exp\left(-\frac{mv^2}{2kT}\right) dv \\
 &= \left(\frac{4\pi}{2} \right) \left(\frac{m}{2\pi kT} \right)^{3/2} \left(\frac{2kT}{m} \right)^2 \\
 &= \boxed{\sqrt{\frac{8kT}{\pi m}} = \sqrt{\frac{8RT}{\pi M}} = \frac{2}{\sqrt{\pi}} v_p} \tag{1.73}
 \end{aligned}$$

The mean square speed $\langle v^2 \rangle$ is the second-order raw moment of the speed distribution. The root mean square speed v_{rms} is the square root of the mean square speed, corresponding to the speed of a particle with median kinetic energy. From $I_4 = \int_0^\infty x^4 e^{-ax^2} dx = \frac{3}{8a^2} \sqrt{\frac{\pi}{a}}$ we can get

$$\begin{aligned}
 v_{\text{rms}} &= \sqrt{\langle v^2 \rangle} = \left(\int_0^\infty v^2 f(v) dv \right)^{1/2} \\
 &= \left(\int_0^\infty \left(\frac{m}{2\pi kT} \right)^{3/2} (4\pi v^4) \exp\left(-\frac{mv^2}{2kT}\right) dv \right)^{1/2} \\
 &= \left(\frac{3\pi}{2} \right) \left(\frac{m}{2\pi kT} \right)^{3/2} \left(\frac{2kT}{m} \right)^2 \left(\frac{2k\pi T}{m} \right)^{1/2} \\
 &= \boxed{\sqrt{\frac{3kT}{m}} = \sqrt{\frac{3RT}{M}} = \sqrt{\frac{3}{2}} v_p} \tag{1.74}
 \end{aligned}$$

In D -dimensional space, according the Maxwell-Boltzman distribution, the root-mean-square speed

$$v_{\text{rms}} = \sqrt{\langle v^2 \rangle} = \left(\frac{DkT}{m} \right)^{1/2} \quad [8].$$

The speed distribution for the molecules of an ideal gas can be illustrated in Fig 1.2. Fig 1.2 also indicates the calculation equations for different of velocities.

1.3.4 Ideal Gas Law

People are often confused by the units of the ideal gas constant. This confusion is compounded by the fact that there are two forms of the gas constant: the universal gas constant and the specific gas constant. To avoid confusion and error, these are defined below, along with their relationships with molar mass and molecular mass. For completeness, numerical values are given in SI units.

A mol amount of matter. Specifically one mol is $6.02214076 \times 10^{23}$ molecules of a substance, a standard number of molecules known as Avogadro number. Strictly speaking, mol does not have dimensions of mass; rather, mol is a primary dimension in and of itself, i.e., the amount of matter. Note that some authors, however, treat mol as a unit of mass.

The mass of 1 mol of substance is designated as molar mass. By definition, the molar mass has the units of grams per mole (g/mol). Molar mass M can be obtained from standard periodic charts or periodic tables of the elements.

For example, the molar mass of oxygen is 16 g/mol. The molar mass of an element is calculated by multiplying the element's relative atomic mass by the molar mass constant of 1 g/mol. When oxygen's atomic mass of 16 is multiplied by the molar mass constant, the result equals 16 g/mol. While elemental oxygen has a molar mass of 16, oxygen often exists bound to another oxygen. In this case, the molar mass of O_2 would be 32.

Another example, molar mass of water is 18 g/mol. One mole of H_2O is made up of 2 moles of hydrogen atoms and 1 mole of oxygen atom. Molar mass of 1 mole of hydrogen atoms is 1 g/mol; molar mass of oxygen is 16 g/mol. Thus, molar mass of H_2O is $2 \text{ g/mol} + 16 \text{ g/mol} = 18 \text{ g/mol}$. Another example, the molar mass of nitrogen is 14.0067 g/mol. Nitrogen in its gaseous or vapor state occurs as a diatomic molecule N_2 ; thus, molar mass of gaseous nitrogen is 28.0134 g/mol. Since air is made up predominantly of nitrogen gas, the molecular weight of air is very close to that of nitrogen, thus molar mass of air $M_{air} = 28.97 \text{ g/mol}$.

1.3.4.1 Common Form

The ideal gas law, also called the general gas equation, is the equation of state of a hypothetical ideal gas. It is a good approximation of the behavior of many gases under many conditions, although it has several limitations. The common form of ideal gas law is written as

$$pV = nRT = NkT \quad (1.75)$$

where p is the pressure of the gas, V is the volume of the gas, T is the absolute temperature of the gas, n is the amount of substance of gas also known as number of moles of gas, N is the number of gas molecules (or the Avogadro constant times the amount of substance $N_A n$), k is the Boltzmann constant, and R is the ideal gas constant, it is the same for all gases.

In SI units, p is measured in pascals, V is measured in cubic meters, n is measured in moles, N is dimensionless, and T in kelvins (the Kelvin scale is a shifted Celsius scale, where $0.00 \text{ K} = -273.15^\circ \text{C}$, the lowest possible temperature).

1.3.4.2 Molar Form

How much gas is present could be specified by giving the mass instead of the chemical amount of gas. Therefore, an alternative form of the ideal gas law may be useful. The chemical amount n (in moles) is equal to total mass of the gas m_t (in grams) divided by the molar mass M (in grams per

mole): $n = \frac{m_t}{M}$.

By replacing n with m_t/M and subsequently introducing density $\rho = \frac{m_t}{V}$, we get:

$$pV = \frac{m_t}{M}RT \Rightarrow p = \frac{m_t}{V} \frac{RT}{M} = \rho \frac{R}{M} T \quad (1.76)$$

Or by replacing N with m_t/m and subsequently introducing density $\rho = \frac{m_t}{V}$, we get:

$$pV = \frac{m_t}{m}kT \Rightarrow p = \frac{m_t}{V} \frac{kT}{m} = \rho \frac{k}{m} T \quad (1.77)$$

Defining the specific gas constant R_{specific} as the ratio R/M ,

$$\boxed{p = \rho R_{\text{specific}} T} \quad (1.78)$$

This form of the ideal gas law is very useful because it links pressure, density, and temperature in a unique formula independent of the quantity of the considered gas. It is common, especially in engineering and meteorological applications, to represent the specific gas constant by the symbol R . In such cases, the universal gas constant is usually given a different symbol such R^* to distinguish it. In any case, the context and/or units of the gas constant should make it clear as to whether the universal or specific gas constant is being referred to.

The gas constant or universal gas constant R is, as its name implies, universal, i.e., the same regardless of the gas being considered. In SI units, it is approximately $8.3143 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$.

The specific gas constant R_{specific} is not universal, and its value depends on the specific gas being considered. R_{specific} is defined as the universal gas constant R divided by the molecular weight of the substance, $R_{\text{specific}} = R/M$. For air in S.I. units, and refer to molar mass of air $M_{\text{air}} = 28.97 \text{ g}\cdot\text{mol}^{-1}$, we can calculate the specific gas constant of air R_{air}

$$\begin{aligned} R_{\text{air}} &= \frac{R}{M_{\text{air}}} = \frac{8.3143 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}}{28.97 \text{ g}\cdot\text{mol}^{-1}} \\ &= 287 \text{ J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1} = 287 \text{ N}\cdot\text{m}\cdot\text{kg}^{-1}\cdot\text{K}^{-1} = 287 \text{ Pa}\cdot\text{m}^3\cdot\text{kg}^{-1}\cdot\text{K}^{-1} \end{aligned}$$

The density of dry air can be calculated using the ideal gas law, expressed as a function of temperature and pressure [15]:

$$\rho = \frac{p}{R_{\text{specific}} T} \quad (1.79)$$

in which ρ is air density in $\text{Pa}\cdot\text{m}^{-3}$, p is absolute pressure in Pa, T is absolute temperature in K, and R_{specific} is specific gas constant for dry air in $\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$.

1.3.4.3 Energy Associated With Ideal Gas

Now we prove the relation of pressure and temperature with kinetic energy [16].

In kinetic model of gases, the pressure is equal to the force exerted by the atoms hitting and rebounding from a unit area of the gas container surface. Consider a gas of N molecules, each of mass m , enclosed in a cube of volume $V = L^3$. When a gas molecule collides with the wall of the container perpendicular to the x axis and bounces off in the opposite direction with the same speed (an elastic collision), the change in momentum is given by:

$$\Delta p = p_{i,x} - p_{f,x} = p_{i,x} - (-p_{i,x}) = 2p_{i,x} = 2mv_x$$

where p is the momentum, i and f indicate initial and final momentum (before and after collision), x indicates that only the x direction is being considered, and v is the speed of the particle (which is the same before and after the collision). The particle impacts one specific side wall once every

$$\Delta t = \frac{2L}{v_x}$$

where L is the distance between opposite walls. The force due to this particle is

$$F = \frac{\Delta p}{\Delta t} = \frac{mv_x^2}{L}$$

The total force on the wall is

$$F = \frac{\Delta p}{\Delta t} = \frac{Nm\overline{v_x^2}}{L}$$

where the bar denotes an average over the N particles.

Since the motion of the particles is random and there is no bias applied in any direction, the average squared speed in each direction is identical:

$$\overline{v_x^2} = \overline{v_y^2} = \overline{v_z^2}$$

In three dimensions the total squared speed $\overline{v^2}$ is given by

$$\overline{v^2} = \overline{v_x^2} + \overline{v_y^2} + \overline{v_z^2}$$

Therefore:

$$\overline{v_x^2} = \frac{\overline{v^2}}{3}$$

And the force can be written as:

$$F = \frac{Nm\overline{v^2}}{3L}$$

This force is exerted on an area L^2 . Therefore, the pressure of the gas is

$$p = \frac{F}{L^2} = \frac{Nm\overline{v^2}}{3V}$$

where $V = L^3$ is the volume of the box.

In terms of the kinetic energy of the gas e :

$$\boxed{pV = \frac{2}{3} \left(\frac{1}{2} Nm\overline{v^2} \right) = \frac{2}{3} e} \quad (1.80)$$

This is a first non-trivial result of the kinetic theory because it relates pressure, a macroscopic property, to the (translational) kinetic energy of the molecules $e = \frac{1}{2} Nm\overline{v^2}$, which is a microscopic

property. Note that from the root mean square speed defined in (1.74), we can also derive that $pV = \frac{Nmv_{\text{rms}}^2}{3}$. This indicates that total squared speed $\overline{v^2}$ has the same meaning of the mean square speed $\langle v^2 \rangle$.

Up to now in the derivation process, there is no assumption that the gas is an ideal gas.

For ideal gas, from the ideal gas law in molar form $p = \rho R_{\text{specific}} T = \rho \frac{R}{M} T$ shown in Eq. (1.78), combine with $e = \frac{3}{2} nRT$ we can derive that

$$p = \frac{2}{3} \frac{\rho e}{nM} \quad (1.81)$$

with M the molar gas. Since the total mass of the gas $m_t = nM$, thus the $\frac{\rho}{nM} = \frac{1}{V}$, with V the volume of the gas, so we can recover $pV = \frac{2}{3} e$. We can summarize the relation between kinetic energy and pressure, as

$$e = \frac{3}{2} pV = \frac{3}{2} \frac{nM}{\rho} p \quad (1.82)$$

For ideal gas, we can also derive the relation between temperature and kinetic energy. Rewriting the above result for the pressure as $pV = \frac{Nmv^2}{3}$, we may combine it with the ideal gas law $pV = nRT = NkT$ shown in Eq. (1.75), with k the Boltzmann constant, R is the gas constant, and T the absolute temperature defined by the ideal gas law, which leads to

$$e = \frac{3}{2} nRT = \frac{3}{2} NkT \quad (1.83)$$

Thus, the kinetic energy e to be identified with the internal energy.

Also, we can find the simplified expression of the average kinetic energy per molecule,

$$\frac{1}{2} m \overline{v^2} = \frac{3}{2} kT \quad (1.84)$$

The kinetic energy of the system is N times that of a molecule, namely $e = \frac{1}{2} N m \overline{v^2}$. Then the temperature T takes the form

$$T = \frac{m \overline{v^2}}{3k} = \frac{2}{3} \frac{e}{Nk} = \frac{2}{3} \frac{e}{nR} \quad (1.85)$$

since $N = N_A n$ and $R = N_A k$ from Definition 1.3.4, thus $nR = nN_A k = Nk$. We obtained one important result of the kinetic theory: The average molecular kinetic energy is proportional to the ideal gas law's absolute temperature.

Since there are $3N$ degrees of freedom in a monatomic-gas system with N particles, the kinetic energy per degree of freedom per molecule is

$$\left(\frac{e}{3N} \right) = \frac{kT}{2} = \frac{RT}{2N_A} \quad (1.86)$$

In the kinetic energy per degree of freedom, the constant of proportionality of temperature is $\frac{k}{2}$ or $\frac{R}{2}$ per mole.

Definition 1.3.6 – Kinetic energy. According to assumptions of the kinetic theory of ideal gases [17], we assume that there are no intermolecular attractions between the molecules of an ideal gas. In other words, its potential energy is zero. Hence, all the energy possessed by the gas is in the kinetic energy of the molecules of the gas $e = \frac{3}{2}nRT = \frac{3}{2}NkT$, in which n is the amount of substance of gas also known as number of moles of gas, N is the number of gas molecules (or the Avogadro constant times the amount of substance $N_A n$). This is the kinetic energy of n moles (with totally N molecules) of a monatomic gas having 3 degrees of freedom; x, y, z . Thus, energy associated with one mole of a monatomic gas $e = \frac{3}{2}RT$; energy associated with one molecule (or atom) of a monatomic gas $e = \frac{3}{2}kT$.

We can see that for each degree of freedom of one mole of a monatomic gas, the kinetic energy which is $RT/2$. Typically, these degrees of freedom are molecular translation, vibration, and rotation. But for monatomic gases, there is no inner molecular structure and there can be no vibration or rotation, leaving only the translational movement in the three spatial dimensions [1]. Thus the internal energy equal the kinetic energy for ideal monatomic gases, i.e. for ideal monatomic gases the internal energy consists of translational energy only.

1.3.4.4 Heat Capacities of Gases

Heat capacity or thermal capacity is a physical property of matter, defined as the amount of heat to be supplied to a given mass of a material to produce a unit change in its temperature. The SI unit of heat capacity is *joule per kelvin* ($\text{J}\cdot\text{K}^{-1}$) [18].

Definition 1.3.7 – Heat capacity. The heat capacity of an object, denoted by C , is the limit

$$C = \lim_{\Delta T \rightarrow 0} \frac{\Delta Q}{\Delta T} \quad (1.87)$$

where ΔQ is the amount of heat that must be added to the object (of mass M) in order to raise its temperature by ΔT .

The value of this parameter usually varies considerably depending on the starting temperature T of the object and the pressure p applied to it. Therefore, it should be considered a function $C(p, T)$ of those two variables. However, the variation can be ignored in contexts when working with objects in narrow ranges of temperature and pressure.

Now we discuss the **heat capacities for a homogeneous system undergoing different thermodynamic processes.**

At constant pressure, $dQ = dU + W = dU + pdV$ (Isobaric process)

At constant pressure, heat supplied to the system would contribute to both the work done and the change in internal energy, according to the first law of thermodynamics. The heat capacity would be called C_p .

At constant volume, $V = 0, dQ = dU + W = dU$ (Isochoric process)

A system undergoing a process at constant volume would imply that no work would be done, so the heat supplied would contribute only to the change in internal energy. The heat capacity obtained this way is denoted C_V . The value of C_V is always less than the value of C_p .

Calculating C_p and C_V for an ideal gas

$$C_p - C_V = nR \quad (1.88a)$$

$$\gamma = C_p/C_V \quad (1.88b)$$

where n is the number of moles of the gas, R is the universal gas constant, and γ is the heat capacity ratio (can be calculated by knowing the degrees of freedom of the gas molecule).

Using the above two relations, the specific heats can be deduced as follows:

$$C_p = \gamma \frac{nR}{\gamma - 1} \quad (1.89a)$$

$$C_V = \frac{nR}{\gamma - 1} \quad (1.89b)$$

At constant temperature (Isothermal process) No change in internal energy (as the temperature of the system is constant throughout the process) leads to only work done of the total supplied heat, and thus infinite amount of heat is required to increase the temperature of the system by a unit temperature, leading to infinite or undefined heat capacity of the system.

We are now deriving these relations.

The value of the heat capacity depends on whether the heat is added at constant volume, constant pressure, etc. The heat capacity at constant pressure C_p is greater than the heat capacity at constant volume C_V , because when heat is added at constant pressure, the substance expands and work.

When heat is added to a gas at constant volume, applying the **First Law of Thermodynamics** and because no work is done ($W = 0$), we have

$$Q_V = C_V \Delta T = \Delta U + W = \Delta U$$

where ΔU denotes the change in the internal energy of a closed system, Q denotes the quantity of energy supplied to the system as heat (Q_V is the heat added to a gas at constant volume), and W denotes the amount of thermodynamic work done by the system on its surroundings.

Therefore,

$$dU = C_V dT \quad \text{and} \quad C_V = \frac{dU}{dT}$$

When heat is added at constant pressure, we have

$$Q_p = C_p \Delta T = \Delta U + W = \Delta U + p \Delta V$$

For infinitesimal changes this becomes

$$C_p dT = dU + p dV = C_V dT + p dV$$

From the ideal gas law, $pV = nRT$ shown in Eq. (1.75), we get for constant pressure

$$d(pV) = pdV + Vdp = p dV = nRdT$$

Substituting this in the previous equation gives

$$C_p dT = C_V dT + nRdT$$

Dividing dT out, we get

$$\boxed{C_p = C_V + nR}$$

For an ideal gas, the heat capacity at constant pressure is greater than that at constant volume by the amount nR .

As discussed, for an ideal monatomic gas the internal energy consists of translational energy only, $U = \frac{3}{2}nRT$. The heat capacities are then

$$C_V = \frac{dU}{dT} = \frac{3}{2}nR = \frac{3}{2}Nk \quad (1.90a)$$

$$C_p = C_V + nR = \frac{5}{2}nR = \frac{5}{2}Nk \quad (1.90b)$$

since $N = N_A n$ and $R = N_A k$ from Definition 1.3.4, thus $nR = nN_A k = Nk$. This is part of the **Equipartition Theorem** [19].

From the relation between the internal energy and the temperature shown in Eq. (1.83), $U = \frac{3}{2}nRT = \frac{3}{2}NkT$, we can derive the equation of state for internal energy as:

$$U = C_V T \quad (1.91)$$

Or we can say that in case of an ideal gas, we can derive that $dU = C_V dT$, i.e. the internal energy of an ideal gas can be written as a function that depends only on the temperature.

So the heat capacity ratio can be obtained for ideal gas as $\gamma = C_p/C_V = 5/3$.

The heat capacity ratio (γ) for an ideal gas can be related to the degrees of freedom (f) of a molecule by

$$\gamma = 1 + \frac{2}{f} \quad (1.92)$$

Thus we observe that for a monatomic gas, with 3 degrees of freedom:

$$\gamma = \frac{5}{3} = 1.6666\dots, \quad (1.93)$$

while for a diatomic gas, with 5 degrees of freedom (at room temperature: 3 translational and 2 rotational degrees of freedom; the vibrational degree of freedom is not involved, except at high temperatures):

$$\gamma = \frac{7}{5} = 1.4 \quad (1.94)$$

For example, the terrestrial air is primarily made up of diatomic gases (around 78% nitrogen, N_2 , and 21% oxygen, O_2), and at standard conditions it can be considered to be an ideal gas. The

above value of 1.4 is highly consistent with the measured adiabatic indices for dry air within a temperature range of 0 – 200 °C, exhibiting a deviation of only 0.2%.

1.3.5 Speed of Sound in Ideal Gas

1.3.5.1 Introduction

The speed of sound in mathematical notation is conventionally represented by c , from the Latin *celeritas* meaning “velocity” [20].

The ideal gas law shown in Eq. (1.78) does not completely express how a variation of one variable of state influences the other. If, for example, the volume of a gas is compressed (by pressing a piston into a vessel), it is also possible that the temperature or the pressure can change. The ideal gas law does not include that detailed information. It only states that the ratio of the two quantities is altered. Additional observations are needed to clarify this.

Experience shows that the speed of the compression and the environment in which the compression takes place are of major importance. If the compression is done very quickly in a piston (or in an insulated environment without thermal conduction) then a temperature increase in the gas can be observed. Usually, thermal conduction is a very slow process that takes a long time (and is even impossible in a thermally non-conducting, insulated environment). Therefore, the observed increase in temperature is not achieved by heat consumed by the exterior, but rather, only results from the interior compression. If the volume compression is done very slowly and takes place in an environment with good thermal conduction, so that a temperature difference between the interior and the exterior can be compensated, the inner temperature can stay constant. In other words, thermal conduction is a crucial prerequisite for isothermal compression [21].

As already mentioned, thermal conduction is a slow process. Thus, isothermal compensations take a long time. In contrast, sound fields are subject to fast changes (apart from the lowest frequencies). It can, therefore, be assumed that sound-related processes happen without the participation of thermal conduction in the gas. In other words, when dealing with sound fields the gas can (nearly) always be assumed to lack thermal conduction. Thermal transportation processes play a minor role. This change in the gaseous state without thermal conduction is called “adiabatic”. The fact that sound related processes are adiabatic also means that they cannot be isothermal, which would imply that thermal conduction takes place. The temperature of the gas and likewise the pressure and the density must therefore be subject to changes in time and space. Apart from scaling factors, these three variables of state even have the same time- and space-dependence, as will be shown shortly.

Definition 1.3.8 – Isothermal process. An isothermal process is a change of a system, in which the temperature remains constant: $\Delta T = 0$. This typically occurs when a system is in contact with an outside thermal reservoir (heat bath), and the change in the system will occur slowly enough to allow the system to continue to adjust to the temperature of the reservoir through heat exchange. In contrast, an adiabatic process is where a system exchanges no heat with its surroundings ($Q = 0$). In other words, in an isothermal process, the value $\Delta T = 0$ and therefore the change in internal energy $\Delta U = 0$ (only for an ideal gas) but $Q \neq 0$, while in an adiabatic process, $\Delta T \neq 0$ but $Q = 0$.

Simply, we can say that in isothermal processes

- $T = \text{constant}$
- $\Delta T = 0$

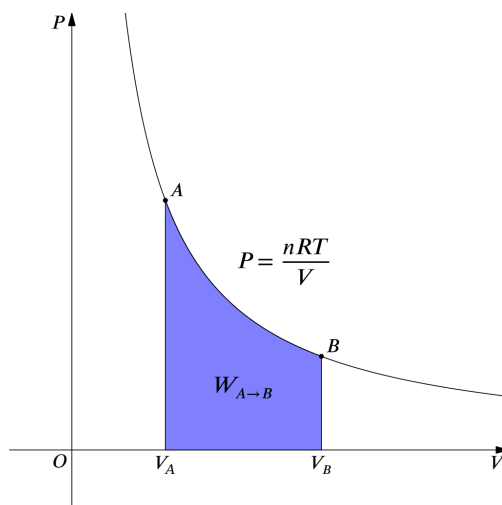


Figure 1.3: Pressure Volume Diagram of an Isothermal Process

- $dT = 0$

while in adiabatic processes

- $Q = 0$

Isothermal refers to a process in which a system changes-whether it be the pressure, volume and/or contents-without the temperature changing. From the point of view of the first law of thermodynamics, this means that the internal energy of the system is unchanged, since temperature is a measure of the average kinetic energy of molecules within the system (for ideal gas, the internal energy is proportional to the temperature, refer to Eq. (1.91)). This then looks like:

$$\Delta U = Q - W = 0 \quad (1.95)$$

and consequently,

$$Q = W \quad (1.96)$$

where ΔU is the change in internal energy, Q is heat, W is work. All the heat added to the system is used to do work.

For an ideal gas, from the ideal gas law shown in Eq. (1.75), $pV = nRT$, where n is the number of moles of gas. Therefore:

$$p = \frac{nRT}{V} = \frac{\text{constant}}{V} \quad (1.97)$$

In thermodynamics, the reversible work involved when a gas changes from state A to state B is

$$W_{A \rightarrow B} = - \int_{V_A}^{V_B} p dV \quad (1.98)$$

For an isothermal, reversible process, this integral equals the area under the relevant pressure-volume isotherm, and is indicated in purple in Fig. 1.3 for an ideal gas.

By convention, work is defined as the work on the system by its surroundings. If, for example, the system is compressed, then the work is positive and the internal energy of the system increases.

Conversely, if the system expands, it does work on the surroundings and the internal energy of the system decreases.

Definition 1.3.9 – Adiabatic process. An adiabatic process occurs without transfer of heat or mass of substances between a thermodynamic system and its surroundings [22]. In an adiabatic process, energy is transferred to the surroundings only as work. Some chemical and physical processes occur so rapidly that they may be conveniently described by the term “adiabatic approximation”, meaning that there is not enough time for the transfer of energy as heat to take place to or from the system.

A process that does not involve the transfer of heat or matter into or out of a system, so that $Q = 0$, is called an adiabatic process, and such a system is said to be adiabatically isolated. The assumption that a process is adiabatic is a frequently made simplifying assumption. For example, the compression of a gas within a cylinder of an engine is assumed to occur so rapidly that on the time scale of the compression process, little of the system’s energy can be transferred out as heat to the surroundings. Even though the cylinders are not insulated and are quite conductive, that process is idealized to be adiabatic. The same can be said to be true for the expansion process of such a system.

The assumption of adiabatic isolation of a system is a useful one, and is often combined with others so as to make the calculation of the system’s behavior possible. Such assumptions are idealizations. The behavior of actual machines deviates from these idealizations, but the assumption of such “perfect” behavior provide a useful first approximation of how the real world works. According to Laplace, when sound travels in a gas, there is no time for heat conduction in the medium and so the propagation of sound is adiabatic. For such an adiabatic process, the modulus of elasticity (Young’s modulus) can be expressed as $E = \gamma p$, where γ is the ratio of specific heats at constant pressure and at constant volume ($\gamma = C_p/C_V$) and p is the pressure of the gas.

Why there is a temperature change in adiabatic process?

In an adiabatic process the heat of the system remains constant. So it is hard to understand that temperature changes in an adiabatic process.

Temperature of gases changes only when internal energy of the gases changes.

Remember adiabatic process implies process in which no heat exchange takes place between the system and the surrounding, i.e. neither heat is supplied nor heat is loosed, $Q = 0$. Since $dU = Q - W$, so any amount of work you do, dU becomes negative of that work you perform to maintain $Q = 0$. Temperature of the gas is related to internal energy by $dU = C_V dT$ (refer to Eq. (1.91)). So in an adiabatic process, if you performed work, then dU has to change, hence temperature also changes.

Definition 1.3.10 – Isentropic process. In thermodynamics, an isentropic process is an idealized thermodynamic process that is both adiabatic^a and reversible. The work transfers of the system are frictionless, and there is no transfer of heat or matter. Such an idealized process is useful in engineering as a model of and basis of comparison for real processes.

^aAn adiabatic process occurs without transfer of heat or mass of substances between a thermodynamic system and its surroundings. In an adiabatic process, energy is transferred to the surroundings only as work.

The first law of thermodynamics provides the basic definition of internal energy, associated with all thermodynamic systems, and states the rule of conservation of energy. The second law [23] is concerned with the direction of natural processes. It asserts that a natural process runs only in one

sense, and is not reversible. For example, heat always flows spontaneously from hotter to colder bodies, and never the reverse, unless external work is performed on the system. The explanation of such phenomena was given in terms of entropy. Total entropy (S) can never decrease over time for an isolated system because the entropy of an isolated system spontaneously evolves toward thermodynamic equilibrium: the entropy should stay the same or increase .

In a fictive reversible process, an infinitesimal increment in the entropy (dS) of a system is defined to result from an infinitesimal transfer of heat (δQ) to a closed system (closed system allows the entry or exit of energy - but not mass transfer) divided by the common temperature (T) of the system in equilibrium and the surroundings which supply the heat:

$$dS = \frac{\delta Q}{T} \quad (\text{closed system, idealized fictive reversible process}) \quad (1.99)$$

Different notations are used for infinitesimal amounts of heat (δ) and infinitesimal amounts of entropy (d) because entropy is a function of state, while heat, like work, is not. The equal sign refers to a reversible process, which is an imagined idealized theoretical limit, never actually occurring in physical reality, with essentially equal temperatures of system and surroundings. For an **isentropic process**, which by definition is reversible, there is no transfer of energy as heat because the process is adiabatic, $\delta Q = 0$. In an irreversible process of transfer of energy as work, entropy is produced within the system; consequently, in order to maintain constant entropy within the system, energy must be removed from the system as heat during the process.

For an actually possible infinitesimal process without exchange of mass with the surroundings, the second law requires that the increment in system entropy fulfills the inequality

$$dS > \frac{\delta Q}{T_{surr}} \quad (\text{closed system, actually possible, irreversible process}) \quad (1.100)$$

This is because a general process for this case may include work being done on the system by its surroundings, which can have frictional or viscous effects inside the system, because a chemical reaction may be in progress, or because heat transfer actually occurs only irreversibly, driven by a finite difference between the system temperature (T) and the temperature of the surroundings (T_{surr}).

In fluid dynamics, an isentropic flow is a fluid flow that is both adiabatic and reversible. That is, no heat is added to the flow, and no energy transformations occur due to friction or dissipative effects. For an isentropic flow of a perfect gas, several relations can be derived to define the pressure, density and temperature along a streamline.

Note that energy can be exchanged with the flow in an isentropic transformation, as long as it doesn't happen as heat exchange. An example of such an exchange would be an isentropic expansion or compression that entails work done on or by the flow.

Derivation of the isentropic relations can be seen as follows.

For a closed system, the total change in energy of a system is the sum of the work done and the heat added:

$$dU = \delta W + \delta Q \quad (1.101)$$

The reversible work done on a system by changing the volume is

$$\delta W = -pdV \quad (1.102)$$

where p is the pressure, and V is the volume. The change in **enthalpy** ($H = U + pV$) is given by

$$dH = dU + pdV + Vdp \quad (1.103)$$

Then for a process that is both reversible and adiabatic (i.e. no heat transfer occurs), $\delta Q_{\text{rev}} = 0$, and so $dS = \delta Q_{\text{rev}}/T = 0$. **All reversible adiabatic processes are isentropic.** This leads to two important observations:

$$dU = \delta W + \delta Q = -pdV + 0 \quad (1.104)$$

$$dH = \delta W + \delta Q + pdV + Vdp = -pdV + 0 + pdV + Vdp = Vdp \quad (1.105)$$

Next, a great deal can be computed for isentropic processes of an ideal gas. For any transformation of an ideal gas, it is always true that (refer to Eq. (1.91))

$$dU = C_V dT, \text{ and } dH = C_p dT \quad (1.106)$$

Using the general results derived above for dU and dH , then

$$dU = C_V dT = -pdV \quad (1.107)$$

$$dH = C_p dT = Vdp \quad (1.108)$$

So for an ideal gas, the heat capacity ratio γ can be written as

$$\gamma = \frac{C_p}{C_V} = -\frac{dp/p}{dV/V} \quad (1.109)$$

For an ideal gas γ is constant. Hence on integrating the above equation, assuming a perfect gas, we get

$$pV^\gamma = \text{constant} \quad (1.110)$$

This is the mathematical equation for an ideal gas undergoing a reversible (i.e., no entropy generation) adiabatic process. This equation can also be represented by the polytropic process equation.

Using the equation of state for an ideal gas $pV = nRT$ we can also derive $TV^{\gamma-1} = \text{constant}$.

Refer to Section 1.3.4.4 for the discussion of the the adiabatic index γ .

Definition 1.3.11 – Polytropic process. A polytropic process is a thermodynamic process that obeys the relation:

$$pV^n = C \quad (1.111)$$

where p is the pressure, V is volume, n is the polytropic index, and C is a constant. The polytropic process equation can describe multiple expansion and compression processes which include heat transfer.

Some specific values of n correspond to particular cases:

- $n = 0$ for an isobaric process^a

- $n = +\infty$ for an isochoric process^b

In addition, when the ideal gas law applies:

- $n = 1$ for an isothermal process^c
- $n = \gamma$ for an isentropic process^d

Where γ is the ratio of the heat capacity at constant pressure (C_p) to heat capacity at constant volume (C_V).

^aAn Isobaric process is a thermodynamic process in which the pressure stays constant: $\Delta p = 0$.

^bAn isochoric process, also called a constant-volume process, an isovolumetric process, or an isometric process, is a thermodynamic process during which the volume of the closed system undergoing such a process remains constant.

^cAn isothermal process is a change of a system, in which the temperature remains constant: $\Delta T = 0$.

^dAn isentropic process is an idealized thermodynamic process that is both adiabatic and reversible. The work transfers of the system are frictionless, and there is no transfer of heat or matter.

In order to determine the speed of sound in a particular medium, we need to know the medium's elastic properties and its density. A medium's elastic properties determine whether or not the medium will deform or lose its shape due to external forces. Sound travels faster in mediums with high elasticity and minimal deformity - like steel. Sound travels more slowly in less rigid mediums that deform easily - like rubber. Sound travels more slowly in mediums with greater density.

Isaac Newton famously considered the speed of sound with a simple formula before most of the development of thermodynamics and so incorrectly used isothermal calculations instead of adiabatic. His result was missing the factor of γ but was otherwise correct. Years later Pierre-Simon Laplace revised Newton's formula and the new formula would be called the Newton-Laplace Equation.

In the latter half of the 17th century, Isaac Newton published his famous work *Principia Mathematica*. Newton thought that he correctly predicted the speed of sound through a medium: solid, liquid, or gas. If he knew the density of the medium and pressure acting on the sound wave, he believed he could ascertain the speed of sound by calculating the square root of the pressure divided by the medium's density:

$$c = \sqrt{\frac{p}{\rho}} \quad (1.112)$$

in which, c is speed of sound, p is pressure acting on the sound, and ρ is density of the medium.

Later in the same century, French mathematician Pierre-Simon Laplace saw the flaw in Newton's thinking and ultimately corrected Newton's formula. He expanded Newton's equation to include the idea that the process is not isothermic as Newton had thought, but it is adiabatic. Laplace slightly revised Newton's formula by adding gamma to Newton's pressure component. Laplace correction:

$$c = \sqrt{\frac{\gamma p}{\rho}} \quad (1.113)$$

Newton's formula neglected the influence of heat on the speed of sound. Laplace made this correction. Experimentation proved that Newton's results were wrong. Results from Newton's equations fell short of what really took place. Laplace's fix hit the mark. A new equation was born: The Newton-Laplace Equations. Laplace shorted the equation by having $K = \gamma p$. K refers to the elastic bulk modulus. The formula is called the Newton-Laplace equation:

$$c = \sqrt{\frac{K}{\rho}} \quad (1.114)$$

We can use this equation to determine the bulk modulus. The speed of sound in sea level atmosphere at 20 °C is $343.21 \text{ m}\cdot\text{s}^{-1}$. Since we know the density of air at sea level is $1.2041 \text{ kg}\cdot\text{m}^{-3}$. We can solve for K .

$$343.21 \text{ m}\cdot\text{s}^{-1} = \sqrt{\frac{K}{1.2041 \text{ kg}\cdot\text{m}^{-3}}} \Rightarrow K \approx 141834 \text{ kg}\cdot\text{m}^{-1}\cdot\text{s}^{-2} = 141834 \text{ Pa}$$

If we know a particular medium's elastic bulk modulus and its density, we can calculate the speed of sound traveling through it. Sound travels faster in mediums with higher elasticity like steel and iron. In mediums like rubber and fiberglass sound travels slower. These mediums easily deform when forces are applied. We can conclude that the sound wave is being attenuated and or absorbed when passing through solids that are easily deformed when a force is applied. The stiffer and less rigid the medium the faster sound will travel through it.

Definition 1.3.12 – Bulk modulus. The bulk modulus (K or B) of a substance is a measure of how resistant to compression that substance is. It is defined as the ratio of the infinitesimal pressure increase to the resulting relative decrease of the volume. Other moduli describe the material's response (strain) to other kinds of stress: the shear modulus describes the response to shear, and Young's modulus describes the response to linear stress. For a fluid, only the bulk modulus is meaningful. For a complex anisotropic solid such as wood or paper, these three moduli do not contain enough information to describe its behavior, and one must use the full generalized Hooke's law.

The bulk modulus $K > 0$ can be formally defined by the equation

$$K = -V \frac{dp}{dV} \quad (1.115)$$

where p is pressure, V is volume, and dp/dV denotes the derivative of pressure with respect to volume. Considering unit mass,

$$K = \rho \frac{dp}{d\rho} \quad (1.116)$$

where ρ is density and $dp/d\rho$ denotes the derivative of pressure with respect to density (i.e. pressure rate of change with volume). The inverse of the bulk modulus gives a substance's compressibility.

Strictly speaking, the bulk modulus is a thermodynamic quantity, and in order to specify a bulk modulus it is necessary to specify how the temperature varies during compression: constant-temperature (isothermal K_T), constant-entropy (isentropic K_S), and other variations are possible. Such distinctions are especially relevant for gases.

For an ideal gas, the isentropic (discussed in Definition 1.3.10) bulk modulus K_S is given by

$$K_S = \gamma p \quad (1.117)$$

and the isothermal bulk modulus K_T is given by

$$K_T = p \quad (1.118)$$

where γ is the heat capacity ratio and p is the pressure.

When the gas is not ideal, these equations give only an approximation of the bulk modulus. In a fluid, the bulk modulus K and the density ρ determine the speed of sound c (pressure waves), according to the Newton-Laplace formula $c = \sqrt{\frac{K}{\rho}}$.

In solids, K_S and K_T have very similar values. Solids can also sustain transverse waves: for these materials one additional elastic modulus, for example the shear modulus G [24], is needed to determine wave speeds.

1.3.5.2 Speed of Sound in Solid

In a three-dimensional solid, there is a non-zero stiffness both for volumetric deformations and shear deformations. Hence, it is possible to generate sound waves with different velocities dependent on the deformation mode. Sound waves generating volumetric deformations (compression) and shear deformations (shearing) are called pressure waves (longitudinal waves) and shear waves (transverse waves), respectively. In earthquakes, the corresponding seismic waves are called P-waves (primary waves) and S-waves (secondary waves), respectively. The sound velocities of these two types of waves propagating in a homogeneous 3-dimensional solid are respectively given by

$$c_{\text{solid,p}} = \sqrt{\frac{K + \frac{4}{3}G}{\rho}} = \sqrt{\frac{E(1 - \nu)}{\rho(1 + \nu)(1 - 2\nu)}} \quad (1.119a)$$

$$c_{\text{solid,s}} = \sqrt{\frac{G}{\rho}} \quad (1.119b)$$

where, K is the bulk modulus of the elastic materials, G is the shear modulus of the elastic materials, E is the Young's modulus, ρ is the density, and ν is Poisson's ratio.

Young's modulus E describes the material's strain response to uniaxial stress in the direction of this stress (like pulling on the ends of a wire or putting a weight on top of a column, with the wire getting longer and the column losing height). the Poisson's ratio ν describes the response in the directions orthogonal to this uniaxial stress (the wire getting thinner and the column thicker). The bulk modulus K describes the material's response to (uniform) hydrostatic pressure (like the pressure at the bottom of the ocean or a deep swimming pool). The shear modulus G describes the material's response to shear stress (like cutting it with dull scissors). The shear modulus is concerned with the deformation of a solid when it experiences a force parallel to one of its surfaces while its opposite face experiences an opposing force (such as friction). These moduli are not independent, and for isotropic materials they are connected via the equations as $2G(1 + \nu) = E = 3K(1 - 2\nu)$ from [24].

Anisotropic materials such as wood, paper and also essentially all single crystals exhibit differing material response to stress or strain when tested in different directions. In this case, one may need to use the full tensor-expression of the elastic constants, rather than a single scalar value.

One possible definition of a fluid would be a material with zero shear modulus.

Note that the speed of pressure waves depends both on the pressure and shear resistance properties of the material, while the speed of shear waves depends on the shear properties only.

Typically, pressure waves travel faster in materials than do shear waves, and in earthquakes this is the reason that the onset of an earthquake is often preceded by a quick upward-downward shock, before arrival of waves that produce a side-to-side motion. For example, for a typical steel alloy, $K = 170 \text{ GPa}$, $G = 80 \text{ GPa}$ and $\rho = 7700 \text{ kg}\cdot\text{m}^{-3}$, yielding a compressional speed $c_{\text{solid,p}}$ of $6000 \text{ m}\cdot\text{s}^{-1}$. This is in reasonable agreement with $c_{\text{solid,p}}$ measured experimentally at $5930 \text{ m}\cdot\text{s}^{-1}$ for a (possibly different) type of steel. The shear speed $c_{\text{solid,s}}$ is estimated at $3200 \text{ m}\cdot\text{s}^{-1}$ using the same numbers.

For one-dimensional solid, the speed of sound for pressure waves in stiff materials such as metals is sometimes given for “long rods” of the material in question, in which the speed is easier to measure. In rods where their diameter is shorter than a wavelength, the speed of pure pressure waves may be simplified and is given by:

$$c_{\text{solid}} = \sqrt{\frac{E}{\rho}} \quad (1.120)$$

where E is Young’s modulus. This is similar to the expression for shear waves, save that Young’s modulus replaces the shear modulus. This speed of sound for pressure waves in long rods will always be slightly less than the same speed in homogeneous 3-dimensional solids, and the ratio of the speeds in the two different types of objects depends on Poisson’s ratio for the material.

1.3.5.3 Speed of Sound in Liquid

For fluids in general, the only non-zero stiffness is to volumetric deformation (a fluid does not sustain shear forces). Hence the speed of sound in a fluid is given by the Newton-Laplace equation:

$$c = \sqrt{\frac{K}{\rho}} \quad (1.121)$$

where K is a coefficient of stiffness, the **isentropic**¹ bulk modulus (or the modulus of bulk elasticity for gases), ρ is the density.

Thus the speed of sound increases with the stiffness (the resistance of an elastic body to deformation by an applied force) of the material and decreases with an increase in density. For ideal gases, the bulk modulus K is simply the gas pressure multiplied by the dimensionless adiabatic index, which is about 1.4 for air under normal conditions of pressure and temperature.

For general equations of state, if classical mechanics is used, the speed of sound c is given by

$$c = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s} \quad (1.122)$$

where p is the pressure, ρ is the density and the derivative is taken isentropically, that is, at constant entropy s .

1.3.5.4 Speed of Sound in Ideal Gas and Air

For an ideal gas, the bulk modulus K is given by

¹In thermodynamics, an isentropic process is an idealized thermodynamic process that is both adiabatic and reversible. Note it not isotropic, isotropic means having properties that are identical in all directions. More details can be found in Definition 1.3.10.

$$K = \gamma \cdot p \quad (1.123)$$

thus, from the Newton-Laplace equation, the speed of sound in an ideal gas is given by

$$c = \sqrt{\gamma \cdot \frac{p}{\rho}} \quad (1.124)$$

where, γ the adiabatic constant (also referred to as the adiabatic exponent, the specific heat ratio, or the isentropic exponent) for the gas. It is the ratio of specific heats of a gas at a constant-pressure to a gas at a constant-volume (c_p/c_v), and arises because a classical sound wave induces an adiabatic compression, in which the heat of the compression does not have enough time to escape the pressure pulse, and thus contributes to the pressure induced by the compression, p is the absolute pressure of the gas, and ρ is the density of the gas.

Using the ideal gas law shown in Eq. (1.78) to replace p with nRT/V , and use $\rho V = m_t = nM$, we have

$$c_{\text{ideal}} = \sqrt{\gamma \cdot \frac{p}{\rho}} = \sqrt{\gamma \cdot \frac{nRT}{\rho V}} = \sqrt{\gamma \cdot \frac{nRT}{m_t}} \quad (1.125)$$

Thus we can derive that,

$$c_{\text{ideal}} = \sqrt{\frac{\gamma RT}{M}} = \sqrt{\gamma R_{\text{specific}} T} = \sqrt{\frac{\gamma kT}{m}} \quad (1.126)$$

where c_{ideal} is the speed of sound in an ideal gas, R (approximately $8.3145 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$) is the molar gas constant (universal gas constant), R_{specific} is the specific gas constant defined as the ratio R/M , k is the Boltzmann constant, γ is the adiabatic index. At room temperature, where thermal energy is fully partitioned into rotation (rotations are fully excited) but quantum effects prevent excitation of vibrational modes, the value is $7/5 = 1.400$ for diatomic molecules, according to kinetic theory. Gamma is actually experimentally measured over a range from 1.3991 to 1.403 at 0°C , for air. Gamma is exactly $5/3 = 1.6667$ for monatomic gases such as noble gases and it is approximately 1.3 for triatomic molecule gases, T is the absolute temperature, M is the molar mass of the gas. The mean molar mass for dry air is about $M_{\text{air}} = 28.97 \text{ g/mol}$, n is the number of moles, m is the mass of a single molecule, and m_t is the total mass of the gas (in grams).

Note that if the ideal gas model is a good model for a real gas, then you can expect, for any specific gas, that there will be no pressure dependence for the speed of sound. This is because as you change the pressure of the gas, you will also change its density by the same factor. The speed of sound will have a very significant dependence on temperature and on the mass of the molecules which make up the gas.

This equation applies only when the sound wave is a small perturbation on the ambient condition. Numerical substitution of the above values gives the ideal gas approximation of sound velocity for gases, which is accurate at relatively low gas pressures and densities (for air, this includes standard Earth sea-level conditions). Also, for diatomic gases the use of $\gamma = 1.4000$ requires that the gas exists in a temperature range high enough that rotational heat capacity is fully excited (i.e., molecular rotation is fully used as a heat energy “partition” or reservoir); but at the same time the temperature must be low enough that molecular vibrational modes contribute no heat capacity (i.e., insignificant heat goes into vibration, as all vibrational quantum modes above the minimum-

energy-mode, have energies too high to be populated by a significant number of molecules at this temperature). For air, these conditions are fulfilled at room temperature, and also temperatures considerably below room temperature (see tables below). Interested readers can investigate in specific heat capacity of gas for a more complete discussion of this phenomenon.

Also stated in [25], a fundamental relation to build the acoustic wave equation is due to the fact that sound in air is an adiabatic phenomenon, which means that there is no local heat exchange².

Now we derive (1.124):

The acoustic quantities represent small time- (and space-) dependent changes which are superimposed on the static quantities. It is thus reasonable to split the total quantities (thus the index *tot*) into a static part and an alternating part. Thus, we write the variables p_{tot} , ρ_{tot} and T_{tot} as the base constant plus the fluctuation p , ρ and T , as

$$p_{tot} = p_0 + p$$

$$\rho_{tot} = \rho_0 + \rho$$

$$T_{tot} = T_0 + T$$

where p_0 , ρ_0 and T_0 are the static quantities “without any sound” and p , ρ and T are the alterations due to the sound field. The superimposed sound field related quantities are designated as sound pressure, sound density and sound temperature. These quantities are actually tiny compared to the static quantities. (Note that here for acoustics quantities, we temporarily use p_{tot} , ρ_{tot} and T_{tot} to represent the total pressure, total density and total pressure; and we temporarily use p_0 , ρ_0 and T_0 to represent the static quantities without any sound, these static quantities should be denoted by p , ρ and T in other places; while here, variables p , ρ and T denote the acoustics quantities.)

When technically quantifying sound pressure, it is more handy to use a logarithmic measure instead of the physical sound pressure itself to represent this wide range. **Sound pressure** (p) is the average variation in atmospheric pressure caused by the sound. Sound pressure is the pressure measured within the wave relative to the surrounding air pressure. Loud sounds produce sound waves with relatively large sound pressures, while quiet sounds produce sound waves with relatively small sound pressures. As the sound pressure increases, the pressure on your eardrum increases as well, making the sound seem louder to you. Sound pressure, like other kinds of pressure, is commonly measured in units of Pascals (Pa). The quietest sound that most people can hear has a sound pressure of 2×10^{-5} Pa, so this pressure is called the threshold of human hearing. The pressure of the sound wave corresponds to how loudly you hear the sound.

Because your ears are sensitive to a very wide range of sound pressure, it makes sense to use a logarithmic scale to measure the loudness of a sound. Sound pressure level uses a logarithmic scale to represent the sound pressure of a sound relative to a reference pressure. The reference sound pressure is typically the threshold of human hearing: : remember that it's 2×10^{-5} Pa.

Sound pressure level (SPL) is measured in units of decibels (dB) and is calculated using the following equation, where p is the sound pressure of the sound wave and p_0 is the reference sound pressure:

²Very near solid walls heat conduction cannot be ignored and process tends to be isothermal, which means that the temperature is constant.

$$L_p = 20 \log_{10} \left(\frac{p}{p_0} \right) \text{ dB} = 10 \log_{10} \left(\frac{p}{p_0} \right)^2 \text{ dB} \quad (1.127)$$

The reference sound pressure p_0 is also denoted as p_{ref} . The reference value p_0 roughly corresponds to the hearing threshold, so that 0 dB denotes the “just perceivable” or “just not perceivable” sound event. The reference sound pressure is $20 \mu\text{Pa} = 20 \times 10^{-6} \text{ N/m}^2$ for sound in air, corresponding roughly to the lowest audible sound at 1 kHz. If not otherwise stated, the sound pressure p stands for the **root mean square** (rms-value) of the time domain signal, also denoted as p_{rms} . The specification in decibels (dB) is not related to a specific unit. It indicates the use of the logarithmic law.

For the sound pressure p , each time it doubles, the SPL will increase 6 dB. This is because

$$L_{p,\text{double}} = 20 \log_{10} 2 \left(\frac{p}{p_0} \right) = 20 \log_{10} \left(\frac{p}{p_0} \right) + 20 \log_{10} (2) \text{ dB} = L_p + 6 \text{ dB} \quad (1.128)$$

For SPL, each increase of 1 dB, the sound pressure (rms-value) will increase 12.3%, this is because $20 \log_{10} (1.123) \approx 1$. For example, if $L_p = 20 \log_{10} \left(\frac{20}{20 \times 10^{-6}} \right) = 20 \log_{10} (10^6) = 120 \text{ dB}$, then we can calculate:

$$L_p = 20 \log_{10} \left(\frac{20 \times 1.123}{20 \times 10^{-6}} \right) = 20 \log_{10} (1.123 \times 10^6) = 121 \text{ dB} \quad (1.129)$$

It should be noted that sound pressures related to the highest sound pressure levels are still remarkably smaller than the static atmospheric pressure of about 10^5 N/m^2 . The rms value of the sound pressure at 140 dB (threshold of pain, hearing loss) is only 200 N/m^2 and therefore 1/500 of atmospheric pressure, since $L_p = 10 \log_{10} \left(\frac{200}{20 \times 10^{-6}} \right)^2 = 10 \log_{10} (10^7)^2 = 140 \text{ dB}$.

When several independent sources of noise are present at the same time the mean square sound pressures generated by the individual sources are additive. This is due to the fact that independent sources generate uncorrelated signals, that is, signals whose instantaneous product average to zero; therefore the cross terms vanish [25]. It follows that

$$p_{\text{rms,tot}}^2 = \sum_i p_{\text{rms},i}^2 \quad (1.130)$$

It is of enormous practical importance that the mean square values of uncorrelated signals are additive, because signals generated by different mechanisms are invariably uncorrelated. Almost all signals that occur in real life are mutually uncorrelated.

The fact that the mean square sound pressures of independent sources are additive leads to the conclusion that the levels of such sources are combined, and the formula for the sum of the sound pressure levels of n incoherent radiating sources is

$$L_{p,\text{tot}} = 10 \log_{10} \left(\frac{p_1^2 + p_2^2 + \cdots + p_n^2}{p_0^2} \right) \text{ dB} \quad (1.131)$$

$$= 10 \log_{10} \left\{ \left(\frac{p_1}{p_0} \right)^2 + \left(\frac{p_2}{p_0} \right)^2 + \cdots + \left(\frac{p_n}{p_0} \right)^2 \right\} \text{ dB} \quad (1.132)$$

Inserting the formulas

$$\left(\frac{p_i}{p_0}\right)^2 = 10^{\frac{L_{p,i}}{10 \text{ dB}}}, \quad i = 1, 2, \dots, n \quad (1.133)$$

in the formula for the sum of the sound pressure levels yields [25, 26]

$$L_{p,tot} = 10 \log_{10} \left(\sum_i 10^{0.1 L_{p,i}} \right) \quad (1.134)$$

The combined sound pressure level of two independent sources: when each of two independent sources in the absence of the other generates a sound pressure level of 70 dB at a certain point, the resulting sound pressure level is 73 dB (not 140 dB!), because $10 \log_{10} (2) \approx 3$. If one source creates a sound pressure level of 65 dB and the other a sound pressure level of 59 dB, the total level is $10 \log_{10} (10^{6.5} + 10^{5.9}) \approx 66$ dB.

If we have three independent sources with the same sound pressure levels, for example, three vehicles with equal sound pressure levels produce a total sound pressure level

$$L_{p,tot} = 10 \log_{10} \left\{ 3 \left(10^{L_{p,i}/10} \right) \right\} = 10 \log_{10} \left(10^{L_{p,i}/10} \right) + 10 \log_{10} (3) = L_i + 4.8 \text{ dB} \quad (1.135)$$

which is 4.8 dB higher than the individual sound pressure level (and not three times higher than the individual sound pressure level).

The **static quantities** as well as the **total quantities**, but not the sound field related quantities alone, because they represent only a part of the total quantity, must certainly fulfill the ideal gas equation in Eq. (1.78) as $p_{tot} = \rho_{tot} R_{\text{specific}} T_{tot}$ or $p_0 = \rho_0 R_{\text{specific}} T_0$.

Thus, from $p_{tot} = \rho_{tot} R_{\text{specific}} T_{tot}$:

$$\begin{aligned} p_0 + p &= (\rho_0 + \rho) R_{\text{specific}} (T_0 + T) \\ &= \rho_0 R_{\text{specific}} T_0 + \rho R_{\text{specific}} T_0 + \rho_0 R_{\text{specific}} T + \rho R_{\text{specific}} T \\ &\approx R_{\text{specific}} (\rho_0 T_0 + \rho_0 T + \rho T_0) \end{aligned}$$

where the (small quadratic) product between sound density and sound temperature (the non-linear high order term $\rho R_{\text{specific}} T$) is neglected. The static quantities vanish, because they are a solution to the ideal gas law themselves, i.e. $p_0 = \rho_0 R_{\text{specific}} T_0$. Divide both sides with the equilibrium state ideal gas equation ($p_0 = \rho_0 R_{\text{specific}} T_0$), we conclude that

$$p = \rho R_{\text{specific}} T_0 + \rho_0 R_{\text{specific}} T \Rightarrow \boxed{\frac{p}{p_0} = \frac{\rho}{\rho_0} + \frac{T}{T_0}} \quad (1.136)$$

If the resulting quotients are designated as “relative quantities”, this equation states that the relative sound pressure is the sum of the relative density and the relative sound temperature.

If air compression/expansion were isothermal (constant temperature T), then according to the ideal gas law in Eq. (1.78) as $p_{tot} = \rho_{tot} R_{\text{specific}} T$, the pressure p_{tot} would simply be proportional to density ρ_{tot} . It turns out, however, that heat diffusion is much slower than audio acoustic vibrations. As a result, air compression/expansion is much closer to **isentropic** (constant entropy s) in normal acoustic situations. (An isentropic process is also called a reversible adiabatic process, as shown

in Definition 1.3.10.) This means that when air is compressed by shrinking its volume V , for example, not only does the pressure p increase, but the temperature T increases as well. In a constant-entropy compression/expansion, temperature changes are not given time to diffuse away to thermal equilibrium. Instead, they remain largely frozen in place. Compressing air heats it up, and relaxing the compression cools it back down.

So if we consider the isentropic process, according to the pressure volume relation shown in Eq. (1.110), we have [22]

$$p_{tot} V_{tot}^\gamma = \text{constant} = p_0 V_0^\gamma \Rightarrow \boxed{\frac{p_{tot}}{p_0} = \left(\frac{V_0}{V_{tot}} \right)^\gamma = \left(\frac{m/\rho_0}{m/\rho_{tot}} \right)^\gamma = \left(\frac{\rho_{tot}}{\rho_0} \right)^\gamma} \quad (1.137)$$

Equation (1.137) describes the relationship between pressure and density in a perfect gas without thermal conduction, since sound fields are subject to fast changes (apart from the lowest frequencies) while thermal conduction is a slow process, as already mentioned. For perfect, diatomic gases, which are of interest in acoustics only, $\gamma = 1.4$.

The second relationship between the sound field quantities is given by the adiabatic equation of state (1.137) which will be adapted for the comparatively small sound field quantities in what follows.

First, note that the adiabatic equation of state (1.137) states a non-linear relationship between pressure and density in the gas. On the other hand, only the smallest alterations around the operating point (p_0, ρ_0) are of interest; thus the curved characteristics can be replaced by its tangent at the operating point. In other words, the characteristics can be linearized, because quadratic and higher order terms of a Taylor series expansion can be neglected.

To do this, the sound field quantities $p_{tot} = p_0 + p$ and $\rho_{tot} = \rho_0 + \rho$ are applied to the specific adiabatic equation for the aggregate values (1.137)

$$\frac{p_0 + p}{p_0} = 1 + \frac{p}{p_0} = \left(\frac{\rho_0 + \rho}{\rho_0} \right)^\gamma = \left(1 + \frac{\rho}{\rho_0} \right)^\gamma \quad (1.138)$$

The power series truncated after the linear term $f(x) = (1 + x)^\gamma$ at $x = 0$ exists in $f(x) = 1 + \gamma x$, therefore

$$1 + \frac{p}{p_0} = \left(1 + \frac{\rho}{\rho_0} \right)^\gamma = 1 + \gamma \frac{\rho}{\rho_0} \quad (1.139)$$

The linearized, adiabatic equation of state adapted for acoustic purposes then becomes

$$\boxed{\frac{p}{p_0} = \gamma \frac{\rho}{\rho_0}} \quad (1.140)$$

Sound fields are nearly always described by means of their pressure distribution, because the sound pressure can be detected with microphones very easily, whereas the sound density can only be determined indirectly by the pressure. So, whenever possible, the sound pressure will be used in the following formulations. For that purpose, if a density occurs it has to be expressed by a sound pressure. This can be achieved by solving (1.140) for the density

$$\rho = \frac{p}{c^2}, \text{ with } c^2 = \gamma \frac{p_0}{\rho_0} \quad (1.141)$$

The introduced constant c has a special physical meaning: c denotes the speed at which the sound propagates in the gas. And for c , the speed of sound in an ideal gas, also shown in Eq. (1.124), we can summarize that [25]

$$c = \sqrt{\frac{p}{\rho}} = \sqrt{\gamma \frac{p_0}{\rho_0}} \quad (1.142)$$

As introduced in Eq. (1.124), p_0 is the absolute pressure of the gas, and ρ_0 is the density of the gas, and they should be static quantities without any sound. Using the ideal gas law shown in Eq. (1.78) we can prove Eq. (1.126), as [21]

$$c = \sqrt{\gamma R_{\text{specific}} T_0} \quad (1.143)$$

Obviously, sound pressure and sound density have the same time and spatial dependence. If the relative density is eliminated in Eq. (1.136) by using Eq. (1.140), the relative sound temperature becomes

$$\frac{T}{T_0} = \frac{p}{p_0} - \frac{\rho}{\rho_0} = \left(1 - \frac{1}{\gamma}\right) \frac{p}{p_0} \quad (1.144)$$

All three relative quantities have the same wave form, apart from different scaling factors.

From the relative quantities in adiabatic process as shown in Eq. (1.136), we can observe that if temperature variation equals zero, $T_{\text{tot}} = T_0 = 0$ and then $p/\rho = p_0/\rho_0$, thereafter

$$\begin{aligned} c &= \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s} = \sqrt{\frac{p}{\rho}} = \sqrt{\frac{p_0}{\rho_0}} \\ &= \sqrt{R_{\text{specific}} T_0} = \sqrt{R_{\text{specific}} T_{\text{tot}}} = \sqrt{\frac{\rho_{\text{tot}} R_{\text{specific}} T_{\text{tot}}}{\rho_{\text{tot}}}} = \sqrt{\frac{p_{\text{tot}}}{\rho_{\text{tot}}}} \end{aligned}$$

From the speed of sound in ideal gas equation in Eq. (1.126), $c_{\text{ideal}} = \sqrt{\gamma R_{\text{specific}} T_0} = \sqrt{\gamma p_0 / \rho_0}$, we conclude that in isothermal process, $\gamma = 1$. This is in accordance with the polytropic process defined in Definition 1.3.11 and the isothermal bulk modulus defined in Definition 1.3.12.

It should perhaps be noted that the assumption of isothermal compression for sound-related processes (which is actually not valid in the unbounded gas) would lead to a speed of sound

$$c_{\text{iso}} = \sqrt{R_{\text{specific}} T_0} = \frac{c_{\text{adia}}}{\sqrt{\gamma}} \approx 0.85 c_{\text{adia}} \quad (1.145)$$

which is too small. As a matter of fact, it was the discrepancy between c_{iso} and experimental values which showed that sound related compression processes are not isothermal but adiabatic. The experimentally determined speed of sound must therefore be equal to c_{adia} .

For comparison the root mean square velocity of the molecules in an ideal gas, an appropriate average for the speed of molecules in the gas, is given by

$$v_{\text{rms}} = \sqrt{\frac{3kT}{m}} \quad (1.146)$$

and since γ is typically between 1.2 and 1.7, you can see that the average speed of the molecules

is closely related to the speed of sound and will be only slightly larger. For typical air at room conditions, the average molecule is moving at about $500 \text{ m}\cdot\text{s}^{-1}$. Note that the speed of sound is largely determined by how fast the molecules move between collisions, and not on how often they make collisions. This is because no energy is lost during the collisions. The collisions do not slow things down but simply randomize the motion - which was already quite random. At higher temperatures the molecules have more energy and are moving faster than at lower temperatures, hence the speed of sound at higher temperatures is faster than at lower temperatures.

Note that from the ideal gas law in Eq. (1.78) as $p_0 = \rho_0 R_{\text{specific}} T_0$ and the speed of sound in ideal gas equation in Eq. (1.126), $c = \sqrt{\gamma R_{\text{specific}} T_0}$, we can derive that $p_0 = \frac{c^2 \rho_0}{\gamma}$. Thus in isothermal process in LBM, $p_0 = c_s^2 \rho_0 = \frac{1}{3} \rho_0$, in which $c_s = \frac{1}{\sqrt{3}}$ is the lattice sound speed as will be discussed in Section 2.1.5.

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Chapter 2 Lattice Boltzmann Fundamentals

2.1 The Distribution Function and Its Moments

2.1.1 The Distribution Function

We have discussed Maxwell's distribution in Eq. (1.49) in Section 1.3.1. Without loss of generality, we consider a fluid system in D -dimensional space. Let \mathbf{x} be the Cartesian coordinates of the configuration space and $\boldsymbol{\xi}$ that of the velocity space.

Refer to Grad [1], the distribution function $F(\mathbf{x}, \boldsymbol{\xi}, t)$ can be defined as the number density of molecules in the $(\mathbf{x}, \boldsymbol{\xi})$. We write $F(\mathbf{x}, \boldsymbol{\xi}, t)$ for the molecular distribution function and $F(\mathbf{x}, \boldsymbol{\xi})d\mathbf{x}d\boldsymbol{\xi}$ for the number of molecules in the physical volume $d\mathbf{x}$ around \mathbf{x} having velocities within $d\boldsymbol{\xi}$ of $\boldsymbol{\xi}$.¹ The function F is usually taken to satisfy the Maxwell-Boltzmann integro-differential equation which will, in principle, determine $F(\mathbf{x}, \boldsymbol{\xi}, t)$ when the initial value $F(\mathbf{x}, \boldsymbol{\xi}, 0)$ is given.

It is convenient to introduce the mass density

$$f(\mathbf{x}, \boldsymbol{\xi}, t) = mF(\mathbf{x}, \boldsymbol{\xi}, t)$$

with m being the mass of a molecule. The element $f d\boldsymbol{\xi}$ represent the mass density of the molecules contained in an infinitesimal velocity element $d\boldsymbol{\xi}$ about the microscopic particle velocity $\boldsymbol{\xi}$. The element of $f d\mathbf{x}d\boldsymbol{\xi}$ represents the total mass of the molecules contained in an element of volume $d\mathbf{x}d\boldsymbol{\xi}$ in phase space. In other words, the distribution function $f(\mathbf{x}, \boldsymbol{\xi}, t)$ represents the density of particles with velocity $\boldsymbol{\xi} = (\xi_x, \xi_y, \xi_z)$ at position \mathbf{x} and time t . In kinetic theory, the distribution function $f(\mathbf{x}, \boldsymbol{\xi}, t)$ is also called the **velocity distribution function** (VDF), which describes the probability density of finding a fictive particle at position \mathbf{x} , time t and with a mesoscopic velocity $\boldsymbol{\xi}$, as mentioned by Coreixas [2].

Since $f(\mathbf{x}, \boldsymbol{\xi}, t)$ simultaneously represents the density of mass in both three-dimensional physical space and in three-dimensional velocity space. Therefore, f has the units

$$[f] = \frac{\text{kg}}{\text{m}^3} \times \frac{1}{(\text{m/s})^3} = \frac{\text{kg} \cdot \text{s}^3}{\text{m}^6} \quad (2.1)$$

2.1.2 Moments of the General Distribution Function

The distribution function f is positive, and we consider its moments with respect to the variable $\boldsymbol{\xi}$. For instance, the **macroscopic mass density** can be found as the zero'th moment

$$\rho(\mathbf{x}, t) = \int f(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi} \quad (2.2)$$

integration being carried over the whole (three-dimensional) velocity space. By integrating over velocity space in this way, we are considering the contribution to the density of particles of all possible velocities at position \mathbf{x} and time t . The function f/ρ is an normalized probability distribution (for example, the Maxwell's distribution $f_v(v)$ shown in Eq. (1.49)). The normalized probability distribution can be obtained using the normalizing constant for a distribution function.

¹The boldface \mathbf{x} is used for vectors, and $d\mathbf{x}$ is used for the three-dimensional volume element.

Definition 2.1.1 – Normalizing constant. In probability theory, a normalizing constant is a constant by which an everywhere non-negative function must be multiplied so the area under its graph is 1, e.g., to make it a probability density function.

$$p(x) = e^{-x^2/2}, \quad x \in (-\infty, \infty) \quad (2.3)$$

Refer to Section 1.3.2 for Gaussian integrals, we have

$$\int_{-\infty}^{\infty} p(x) dx = \int_{-\infty}^{\infty} e^{-x^2/2} dx = \sqrt{2\pi} \quad (2.4)$$

if we define a function $\varphi(x)$ as

$$\varphi(x) = \frac{1}{\sqrt{2\pi}} p(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \quad (2.5)$$

so that

$$\int_{-\infty}^{\infty} \varphi(x) dx = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} dx = 1 \quad (2.6)$$

then the function $\varphi(x)$ is a probability density function. Actually, probability density function $\varphi(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$ describes the **standard normal distribution**. And constant $\frac{1}{\sqrt{2\pi}}$ is the normalizing constant of function $p(x)$.

We can also consider the particles' contribution ξf to the momentum density. Again considering all possible velocities, we find the **macroscopic momentum density** as the moment

$$\rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) = \int \xi f(\mathbf{x}, \xi, t) d\xi \quad (2.7)$$

The distribution function, f , and therefore all its moments, is a continuous point function; we proceed to interpret these moments physically. The function f is the mass density in (\mathbf{x}, ξ) space; consequently, $\rho = \int f d\xi$ is the mass density in the physical space. In particular, $\rho(\mathbf{x}, t)$ is a smooth point function despite the molecular graininess [1].

The mean value of ξ ,

$$\mathbf{u}(\mathbf{x}, t) = \frac{1}{\rho} \int \xi f(\mathbf{x}, \xi, t) d\xi \quad (2.8)$$

is defined to be the macroscopic flow velocity; $\xi f d\xi$ is an *element of momentum*, therefore it follows that $\rho \mathbf{u}$ is the momentum per unit volume.

Similarly, we can find the **macroscopic total energy density**² $\rho(\mathbf{x}, t) E(\mathbf{x}, t)$ as the moment

$$\rho(\mathbf{x}, t) E(\mathbf{x}, t) = \frac{1}{2} \int |\xi|^2 f(\mathbf{x}, \xi, t) d\xi \quad (2.9)$$

²Note that $E(\mathbf{x}, t)$ can be seen as the total energy with unit mass, which only depends on squared microscopic particle velocity ξ^2 , while the total energy of a small element with mass Δm and volume Δv should be $\Delta m E(\mathbf{x}, t)$. Thus, the macroscopic total energy density (with respect to the small volume) will be $(\Delta m / \Delta v) E(\mathbf{x}, t) = \rho(\mathbf{x}, t) E(\mathbf{x}, t)$. Following the same rule, the macroscopic internal energy density $\rho(\mathbf{x}, t) E(\mathbf{x}, t)$ can be understood.

It is convenient to introduce a special notation [3]. The N -vector x_i ($i = 1, 2, \dots, N$) is denoted by \mathbf{x} . The second order tensor (dyad) $x_i x_j$ is denoted by \mathbf{x}^2 . Similarly, \mathbf{x}^n is used for the n -th order tensor $x_{i_1} x_{i_2} \cdots x_{i_n}$. For the scalar product

$$\sum_{i=1}^N x_i^2 = x^2 \quad (2.10)$$

The lightface x^2 is used.

Thus, $|\boldsymbol{\xi}|^2 = \boldsymbol{\xi} \cdot \boldsymbol{\xi} = \sum_{i=1}^N \xi_i^2 = \xi^2$ is a dot product or scalar product.

This contains two types of energy; the energy $\frac{1}{2}\rho|\mathbf{u}|^2$ due to the bulk motion of the fluid and the internal energy due to the random thermal motion of the gas particles. It is also possible to find only the latter type, the **macroscopic internal energy density**, as the moment [4]

$$\rho(\mathbf{x}, t)e(\mathbf{x}, t) = \frac{1}{2} \int |\boldsymbol{\xi} - \mathbf{u}(\mathbf{x}, t)|^2 f(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi} = \frac{1}{2} \int |\mathbf{c}(\mathbf{x}, \boldsymbol{\xi}, t)|^2 f(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi} \quad (2.11)$$

These expressions for the fluid energy only consider the translational energy of the molecules, i.e. the energy due to the movement with their velocity $\boldsymbol{\xi}$. In the more difficult kinetic theory of polyatomic gases, the internal energy must include additional degrees of freedom, such as molecular vibrational and rotational energies.

It is convenient to measure all higher moments with respect to the mean, and we introduce the **intrinsic velocity**, which is the deviation of the particle velocity from the local mean velocity:

$$\mathbf{c}(\mathbf{x}, \boldsymbol{\xi}, t) = \boldsymbol{\xi} - \mathbf{u}(\mathbf{x}, t) \quad (2.12)$$

Clearly,

$$\begin{aligned} \int \mathbf{c} f d\boldsymbol{\xi} &= \int \{\boldsymbol{\xi} - \mathbf{u}(\mathbf{x}, t)\} f d\boldsymbol{\xi} \\ &= \int \boldsymbol{\xi} f d\boldsymbol{\xi} - \mathbf{u}(\mathbf{x}, t) \int f d\boldsymbol{\xi} \\ &= \rho \mathbf{u}(\mathbf{x}, t) - \rho \mathbf{u}(\mathbf{x}, t) = 0 \end{aligned} \quad (2.13)$$

The vector notation \mathbf{c} and component notation c_i ($i = x, y, z$) will be used interchangeably. By their definitions, the moments are symmetric in the subscripts. There are six distinct second order moments, ten of the third order, $\frac{1}{2}(n+1)(n+2)$ distinct moments of order n .

With defined intrinsic velocity, the second, third, and fourth moments are defined in Cartesian tensor notation by

$$P_{ij}(\mathbf{x}, t) = \int c_i c_j f d\boldsymbol{\xi} \quad (2.14a)$$

$$Q_{ijk}(\mathbf{x}, t) = \int c_i c_j c_k f d\boldsymbol{\xi} \quad (2.14b)$$

$$R_{ijkl}(\mathbf{x}, t) = \int c_i c_j c_k c_l f d\boldsymbol{\xi} \quad (2.14c)$$

In velocity space $\boldsymbol{\xi}$, \mathbf{u} is constant, since $\mathbf{u}(\mathbf{x}, t)$ is not depend on $\boldsymbol{\xi}$. Thus the integration variable in Eq. (2.11) and Eq. (2.14) $d\boldsymbol{\xi} = d(\mathbf{c} + \mathbf{u}) = d\mathbf{c}$, as adopted by Shan et al. [5].

From the ideal gas law, the temperature is by definition proportional to the mean kinetic energy or the internal energy, measured with respect to the flow velocity, \mathbf{u} , i.e. $e_t = \frac{3}{2}nRT = \frac{3}{2}NkT$, as shown in Eq. (1.83). By replacing n with m_t/M , or replacing N with m_t/m , with n the amount of substance (in moles), N the number of gas molecules, m_t the total mass of the gas (in grams), and M the molar mass (in grams per mole), we have $e_t = \frac{3}{2} \frac{m_t}{M} RT = \frac{3}{2} \frac{m_t}{m} kT = \frac{3}{2} m_t R_{\text{specific}} T$ with R_{specific} the specific gas constant.³ An *element of kinetic energy* is $\frac{1}{2} |\mathbf{c}|^2 f d\mathbf{x} d\boldsymbol{\xi} = \frac{1}{2} c^2 f d\mathbf{x} d\boldsymbol{\xi}$. Here, consider a small mass Δm with volume Δv in the system at location \mathbf{x} , within which the intrinsic velocity \mathbf{c} and distribution f are constants i.e. $\mathbf{c}(\mathbf{x}_c, \boldsymbol{\xi}, t)$ and $f(\mathbf{x}_c, \boldsymbol{\xi}, t)$, in which \mathbf{x}_c denotes conditional constant, which means inside the small volume Δv at \mathbf{x} , \mathbf{c} and f are assumed constant with respect to $d\mathbf{x}$ of \mathbf{x} ; while outside the small volume, \mathbf{c} and f varies with respect to \mathbf{x} . We can integrate the kinetic energy element over the whole space and velocities of this small volume Δv to get the total kinetic energy of the small volume at \mathbf{x} , $\frac{1}{2} \iint |\mathbf{c}(\mathbf{x}_c, \boldsymbol{\xi}, t)|^2 f(\mathbf{x}_c, \boldsymbol{\xi}, t) d\mathbf{x} d\boldsymbol{\xi} = \frac{1}{2} \int d\mathbf{x} \int |\mathbf{c}(\mathbf{x}, \boldsymbol{\xi}, t)|^2 f(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi} = \frac{1}{2} \Delta v \int |\mathbf{c}(\mathbf{x}, \boldsymbol{\xi}, t)|^2 f(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi}$. Therefore

$$e_t = \frac{3}{2} \Delta m R_{\text{specific}} T(\mathbf{x}, t) = \frac{1}{2} \Delta v \int |\mathbf{c}(\mathbf{x}, \boldsymbol{\xi}, t)|^2 f(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi}$$

In other words, the ideal gas law means that the temperature is a certain second moment of the distribution function f . Consider the density of the small volume, $\rho(\mathbf{x}, t) = \Delta m / \Delta v$, we can get

$$\begin{aligned} \frac{3}{2} \frac{\Delta m}{\Delta v} R_{\text{specific}} T(\mathbf{x}, t) &= \frac{3}{2} \rho(\mathbf{x}, t) R_{\text{specific}} T(\mathbf{x}, t) = \frac{3}{2} p(\mathbf{x}, t) \\ &= \frac{1}{2} \int |\mathbf{c}(\mathbf{x}, \boldsymbol{\xi}, t)|^2 f(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi} = \frac{1}{2} \int c_i c_i f d\boldsymbol{\xi} = \frac{1}{2} P_{ii}(\mathbf{x}, t) \end{aligned}$$

From the ideal gas law, the pressure of the gas $p = \rho R_{\text{specific}} T$ defined in Eq. (1.78), we have,

$$P_{ii} = 3p \quad (2.15)$$

Or in D -dimensional space, we have

$$P_{ii} = Dp \quad (2.16)$$

Note that here P_{ii} follows the Einstein summation rule, i.e. for the D -dimensional second rank tensor, $P_{ii} = \text{tr}(P_{ij}) = \sum_{i=1}^D P_{ii}$.

³In this situation, the internal energy with unit mass will be $e = \frac{3}{2} \frac{RT}{M} = \frac{3}{2} \frac{kT}{m}$.

The significance of the complete second moment, P_{ij} , is revealed by noting that $c_i f d\mathbf{x} d\boldsymbol{\xi}$ is an *element of momentum* in the i -direction, and $c_i c_j f d\mathbf{x} d\boldsymbol{\xi}$ is the rate at which the i -component of momentum is transferred in the j -direction. In other words, $P_{ij}(\mathbf{x}, t) = \int c_i c_j f d\boldsymbol{\xi}$ is the contribution to the stress tensor which is due to the momentum transfer resulting from molecular motion.

Show that the total and internal energy densities at a given position and time are related as

$$\rho e = \rho E - \frac{1}{2} \rho |\mathbf{u}|^2 \quad (2.17)$$

First, for the intrinsic velocity

$$|\mathbf{c}(\mathbf{x}, \boldsymbol{\xi}, t)|^2 = |\boldsymbol{\xi} - \mathbf{u}(\mathbf{x}, t)|^2 \quad (2.18)$$

Also, since $|\mathbf{c}|^2 = \mathbf{c} \cdot \mathbf{c}$, and $|\boldsymbol{\xi} - \mathbf{u}|^2 = (\boldsymbol{\xi} - \mathbf{u}) \cdot (\boldsymbol{\xi} - \mathbf{u})$, all involve scalar product, we have

$$|\mathbf{c}|^2 = |\boldsymbol{\xi}|^2 - 2(\boldsymbol{\xi} \cdot \mathbf{u}) + |\mathbf{u}|^2 \quad (2.19)$$

Therefore,

$$\begin{aligned} \rho e &= \frac{1}{2} \int |\mathbf{c}|^2 f d\boldsymbol{\xi} = \frac{1}{2} \int |\boldsymbol{\xi} - \mathbf{u}|^2 f d\boldsymbol{\xi} \\ &= \frac{1}{2} \int (|\boldsymbol{\xi}|^2 - 2(\boldsymbol{\xi} \cdot \mathbf{u}) + |\mathbf{u}|^2) f d\boldsymbol{\xi} \\ &= \rho E - \int (\boldsymbol{\xi} \cdot \mathbf{u}) f d\boldsymbol{\xi} + \frac{1}{2} |\mathbf{u}|^2 \int f d\boldsymbol{\xi} \\ &= \rho E - \left(\int \boldsymbol{\xi} f d\boldsymbol{\xi} \right) \cdot \mathbf{u} + \frac{1}{2} \rho |\mathbf{u}|^2 \\ &= \rho E - \rho \mathbf{u} \cdot \mathbf{u} + \frac{1}{2} \rho |\mathbf{u}|^2 \\ &= \rho E - \frac{1}{2} \rho |\mathbf{u}|^2 \end{aligned} \quad (2.20)$$

2.1.3 Moments of the Equilibrium Distribution Function

In D -dimensional space, the equilibrium distribution becomes:

$$f^{\text{eq}} = \rho \left(\frac{m}{2\pi kT} \right)^{D/2} \exp\left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) = \rho \left(\frac{m}{2\pi kT} \right)^{D/2} \exp\left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) \quad (2.21)$$

where D is the dimension of the space, k is the Boltzmann constant, and m is the mass of the molecule. The mass density ρ , macroscopic fluid velocity \mathbf{u} , and the temperature T , are all functions of \mathbf{x} and t . The function f^{eq}/ρ is the Maxwell's distribution $f_{\mathbf{v}}(v)$ shown in Eq. (1.49) which is an normalized probability distribution. It is easily verified that all odd moments vanish.

Show that the moments in Eq. (2.2), Eq. (2.7), and Eq. (2.11) applied to the equilibrium distribution in Eq. (2.21) will result in a density ρ , a fluid velocity \mathbf{u} and internal energy e .

First, we consider $\int f(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi}$ in Eq. (2.2).

Refer to the Gaussian integral in Definition 1.3.1, $\int_{-\infty}^{\infty} e^{-a(x+b)^2} dx = \sqrt{\frac{\pi}{a}}$, we first consider velocities in x direction ξ_x in a three dimensional velocity space ξ (or in any one of the directions in a D -dimensional velocity space), and in this velocity space the macroscopic velocity \mathbf{u} is constant (not depend on ξ), thus:

$$\begin{aligned} \int f^{\text{eq}}(\mathbf{x}, \xi_x, t) d\xi_x &= \int \left\{ \rho \left(\frac{m}{2\pi kT} \right)^{1/2} \exp \left(-\frac{m(\xi_x - u_x)^2}{2kT} \right) \right\} d\xi_x \\ &= \rho \left(\frac{m}{2\pi kT} \right)^{1/2} \int \exp \left(-\frac{m(\xi_x - u_x)^2}{2kT} \right) d\xi_x \\ &= \rho \left(\frac{m}{2\pi kT} \right)^{1/2} \left(\frac{2\pi kT}{m} \right)^{1/2} = \rho \end{aligned}$$

Thus, for integration in three dimensions (or similar to D dimensions), it's easy to obtain

$$\int f^{\text{eq}}(\mathbf{x}, \xi, t) d\xi = \iiint \left\{ \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left(-\frac{m|\xi - \mathbf{u}|^2}{2kT} \right) \right\} d\xi_x d\xi_y d\xi_z = \rho \quad (2.22)$$

Thus, moments of the equilibrium distribution in Eq. (2.21) can result in density ρ shown in Eq. (2.2).

Note that in this process, $|\xi - \mathbf{u}|^2 = (\xi - \mathbf{u}) \cdot (\xi - \mathbf{u}) = |\xi|^2 - 2(\xi \cdot \mathbf{u}) + |\mathbf{u}|^2$, thus for a three dimensional space

$$\begin{aligned} |\xi - \mathbf{u}|^2 &= (\xi_x^2 + \xi_y^2 + \xi_z^2) - 2(\xi_x u_x + \xi_y u_y + \xi_z u_z) + (u_x^2 + u_y^2 + u_z^2) \\ &= (\xi_x - u_x)^2 + (\xi_y - u_y)^2 + (\xi_z - u_z)^2 \end{aligned}$$

So it's okay to solely use $(\xi_x - u_x)^2$ to represent the component of the squared velocity magnitude $|\xi - \mathbf{u}|^2$ in x direction.

Next, we consider $\int \xi f(\mathbf{x}, \xi, t) d\xi$ in Eq. (2.7).

Note that the Gaussian integral $\int_{-\infty}^{\infty} x e^{-a(x+b)^2} dx = -b \sqrt{\frac{\pi}{a}}$ refer to Definition 1.3.1. For integration in three dimensions (or similar to D dimensions), we have

$$\begin{aligned}
\int \boldsymbol{\xi} f^{\text{eq}}(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi} &= \iiint (\xi_x \mathbf{i}_x + \xi_y \mathbf{i}_y + \xi_z \mathbf{i}_z) f^{\text{eq}}(\mathbf{x}, (\xi_x, \xi_y, \xi_z), t) d\xi_x d\xi_y d\xi_z \\
&= \iiint (\xi_x \mathbf{i}_x + \xi_y \mathbf{i}_y + \xi_z \mathbf{i}_z) \left\{ \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) \right\} d\xi_x d\xi_y d\xi_z \\
&= \mathbf{i}_x \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint \xi_x \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) d\xi_x d\xi_y d\xi_z + \\
&\quad \mathbf{i}_y \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint \xi_y \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) d\xi_x d\xi_y d\xi_z + \\
&\quad \mathbf{i}_z \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint \xi_z \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) d\xi_x d\xi_y d\xi_z
\end{aligned}$$

in which \mathbf{i}_x , \mathbf{i}_y , \mathbf{i}_z are the standard unit vectors in the directions of the x , y and z coordinates, respectively. We first consider the \mathbf{i}_x part.

$$\begin{aligned}
&\mathbf{i}_x \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint \xi_x \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) d\xi_x d\xi_y d\xi_z \\
&= \mathbf{i}_x \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint \xi_x e^{\left\{ -\frac{m(\xi_x - u_x)^2}{2kT} \right\}} e^{\left\{ -\frac{m(\xi_y - u_y)^2}{2kT} \right\}} e^{\left\{ -\frac{m(\xi_z - u_z)^2}{2kT} \right\}} d\xi_x d\xi_y d\xi_z \\
&= \mathbf{i}_x \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \int e^{\left\{ -\frac{m(\xi_x - u_x)^2}{2kT} \right\}} \int e^{\left\{ -\frac{m(\xi_y - u_y)^2}{2kT} \right\}} \int \xi_x e^{\left\{ -\frac{m(\xi_z - u_z)^2}{2kT} \right\}} d\xi_x d\xi_y d\xi_z \\
&= \mathbf{i}_x \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \left\{ \left(\frac{2\pi kT}{m} \right)^{1/2} \right\} \left\{ \left(\frac{2\pi kT}{m} \right)^{1/2} \right\} \left\{ u_x \left(\frac{2\pi kT}{m} \right)^{1/2} \right\} \\
&= \mathbf{i}_x \rho u_x
\end{aligned}$$

Same procedures can be applied to \mathbf{i}_y and \mathbf{i}_z parts, thus we have

$$\int \boldsymbol{\xi} f^{\text{eq}}(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi} = \mathbf{i}_x \rho u_x + \mathbf{i}_y \rho u_y + \mathbf{i}_z \rho u_z = \rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) \quad (2.23)$$

Thus, moments of the equilibrium distribution in Eq. (2.21) can result in fluid velocity \mathbf{u} shown in Eq. (2.7).

Next, we consider $\frac{1}{2} \int |\boldsymbol{\xi}|^2 f(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi}$ in Eq. (2.9).

We will use the Gaussian integral $\int_{-\infty}^{\infty} x^2 e^{-a(x+b)^2} dx = \frac{1}{2a} \sqrt{\frac{\pi}{a}} + b^2 \sqrt{\frac{\pi}{a}}$ refer to Definition 1.3.1. For integration in three dimensions (or similar to D dimensions), we have

$$\begin{aligned}
\frac{1}{2} \int |\boldsymbol{\xi}|^2 f^{\text{eq}} d\boldsymbol{\xi} &= \frac{1}{2} \int |\boldsymbol{\xi}|^2 \left\{ \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) \right\} d\boldsymbol{\xi} \\
&= \frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint \xi_x^2 \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) d\xi_x d\xi_y d\xi_z + \\
&\quad \frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint \xi_y^2 \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) d\xi_x d\xi_y d\xi_z + \\
&\quad \frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint \xi_z^2 \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) d\xi_x d\xi_y d\xi_z
\end{aligned}$$

We consider the ξ_x^2 part first.

$$\begin{aligned}
&\frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint \xi_x^2 \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint \xi_x^2 e^{\left\{ -\frac{m(\xi_x - u_x)^2}{2kT} \right\}} e^{\left\{ -\frac{m(\xi_y - u_y)^2}{2kT} \right\}} e^{\left\{ -\frac{m(\xi_z - u_z)^2}{2kT} \right\}} d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \int e^{\left\{ -\frac{m(\xi_x - u_x)^2}{2kT} \right\}} \int e^{\left\{ -\frac{m(\xi_y - u_y)^2}{2kT} \right\}} \int \xi_x^2 e^{\left\{ -\frac{m(\xi_z - u_z)^2}{2kT} \right\}} d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \left\{ \left(\frac{2\pi kT}{m} \right)^{1/2} \right\} \left\{ \left(\frac{2\pi kT}{m} \right)^{1/2} \right\} \left\{ \left(\frac{kT}{m} + u_x^2 \right) \left(\frac{2\pi kT}{m} \right)^{1/2} \right\} \\
&= \frac{1}{2} \rho \frac{kT}{m} + \frac{1}{2} \rho u_x^2
\end{aligned}$$

Following the same procedures for the ξ_y^2 and ξ_z^2 parts, or consider the symmetries of the integrands, we have

$$\frac{1}{2} \int |\boldsymbol{\xi}|^2 f^{\text{eq}}(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi} = \frac{3}{2} \rho(\mathbf{x}, t) \frac{kT(\mathbf{x}, t)}{m} + \frac{1}{2} \rho |\mathbf{u}(\mathbf{x}, t)|^2 \quad (2.24)$$

According to discussions in Section (2.1.2), $e = \frac{3}{2} \frac{RT}{M} = \frac{3}{2} \frac{kT}{m}$, we have

$$\frac{1}{2} \int |\boldsymbol{\xi}|^2 f^{\text{eq}}(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi} = \rho(\mathbf{x}, t) e(\mathbf{x}, t) + \frac{1}{2} \rho |\mathbf{u}(\mathbf{x}, t)|^2 \quad (2.25)$$

From the relation between total and internal energy densities $\rho e + \frac{1}{2} \rho |\mathbf{u}|^2 = \rho E$ shown in Eq. (2.17), **thus, moments of the equilibrium distribution in Eq. (2.21) can result in total energy E (with unit mass) shown in Eq. (2.9).**

Finally, we consider $\frac{1}{2} \int |\boldsymbol{\xi} - \mathbf{u}(\mathbf{x}, t)|^2 f(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi}$ in Eq. (2.11).

We will use the Gaussian integral $\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{1}{2a} \sqrt{\frac{\pi}{a}}$ refer to Definition 1.3.1. For integration in three dimensions (or similar to D dimensions), we have

$$\begin{aligned}
\frac{1}{2} \int |\boldsymbol{\xi} - \mathbf{u}|^2 f^{\text{eq}} d\boldsymbol{\xi} &= \frac{1}{2} \int |\boldsymbol{\xi} - \mathbf{u}|^2 \left\{ \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) \right\} d\boldsymbol{\xi} \\
&= \frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint (\xi_x - u_x)^2 \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) d\xi_x d\xi_y d\xi_z + \\
&\quad \frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint (\xi_y - u_y)^2 \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) d\xi_x d\xi_y d\xi_z + \\
&\quad \frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint (\xi_z - u_z)^2 \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) d\xi_x d\xi_y d\xi_z
\end{aligned}$$

First, we consider only the $(\xi_x - u_x)^2$ part, and we introduce the intrinsic velocity in x direction, $c_x = \xi_x - u_x$, as discussed in Eq. (2.12), and in velocity space $\boldsymbol{\xi}$, $dc_x = d\xi_x$. Then

$$\begin{aligned}
&\frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint (\xi_x - u_x)^2 \exp \left(-\frac{m|\boldsymbol{\xi} - \mathbf{u}|^2}{2kT} \right) d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \iiint (\xi_x - u_x)^2 e^{\left\{ -\frac{m(\xi_x - u_x)^2}{2kT} \right\}} e^{\left\{ -\frac{m(\xi_y - u_y)^2}{2kT} \right\}} e^{\left\{ -\frac{m(\xi_z - u_z)^2}{2kT} \right\}} d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \int e^{\left\{ -\frac{m(\xi_z - u_z)^2}{2kT} \right\}} \int e^{\left\{ -\frac{m(\xi_y - u_y)^2}{2kT} \right\}} \int (\xi_x - u_x)^2 e^{\left\{ -\frac{m(\xi_x - u_x)^2}{2kT} \right\}} d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \int e^{\left\{ -\frac{m(\xi_z - u_z)^2}{2kT} \right\}} \int e^{\left\{ -\frac{m(\xi_y - u_y)^2}{2kT} \right\}} \int c_x^2 e^{\left\{ -\frac{mc_x^2}{2kT} \right\}} dc_x d\xi_y d\xi_z \\
&= \frac{1}{2} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \left\{ \left(\frac{2\pi kT}{m} \right)^{1/2} \right\} \left\{ \left(\frac{2\pi kT}{m} \right)^{1/2} \right\} \left\{ \frac{kT}{m} \left(\frac{2\pi kT}{m} \right)^{1/2} \right\} \\
&= \frac{1}{2} \rho \frac{kT}{m}
\end{aligned}$$

Following the same procedures for the $(\xi_y - u_y)^2$ and $(\xi_z - u_z)^2$ parts, or consider the symmetries of the integrands, we have

$$\frac{1}{2} \int |\boldsymbol{\xi} - \mathbf{u}(\mathbf{x}, t)|^2 f^{\text{eq}}(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi} = \frac{3}{2} \rho(\mathbf{x}, t) \frac{kT(\mathbf{x}, t)}{m} \quad (2.26)$$

According to discussions in Section (2.1.2), $e = \frac{3}{2} \frac{RT}{M} = \frac{3}{2} \frac{kT}{m}$, we have

$$\frac{1}{2} \int |\boldsymbol{\xi} - \mathbf{u}(\mathbf{x}, t)|^2 f^{\text{eq}}(\mathbf{x}, \boldsymbol{\xi}, t) d\boldsymbol{\xi} = \rho(\mathbf{x}, t) e(\mathbf{x}, t) \quad (2.27)$$

Thus, moments of the equilibrium distribution in Eq. (2.21) can result in internal energy e (with unit mass) shown in Eq. (2.11).

2.1.4 Boltzmann BGK Equation

The evolution of the single-particle distribution function obeys the Boltzmann equation. For simplicity, we describe the analytical formulation based on the BGK collision model. As our starting

point, f satisfies the following Boltzmann-BGK equation in continuous velocity space:

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla f + \mathbf{g} \cdot \nabla_{\boldsymbol{\xi}} f = \Omega_f \quad (2.28)$$

Here, f , $\boldsymbol{\xi}$, and \mathbf{g} are the single-particle distribution, the particle velocity, and the external body force (in a unit of acceleration $\text{m} \cdot \text{sec}^{-2}$), respectively; ∇ is the gradient operator in physical space; $\nabla_{\boldsymbol{\xi}}$ is the gradient operator in velocity space; and Ω_f is the collision operator.

In index notation, the Boltzmann equation in continuous velocity space will be [4]

$$\frac{\partial f}{\partial t} + \xi_{\alpha} \frac{\partial f}{\partial x_{\alpha}} + g_{\alpha} \frac{\partial f}{\partial \xi_{\alpha}} = \Omega_f \quad (2.29)$$

As discussed in Section 2.1.2, the macroscopic quantities of interest (density ρ , momentum $\rho \mathbf{u}$, and total energy ρE) are recovered summing up their mesoscopic counterparts over the velocity space:

$$\rho = \int f d\boldsymbol{\xi} \quad (2.30a)$$

$$\rho \mathbf{u} = \int \boldsymbol{\xi} f d\boldsymbol{\xi} \quad (2.30b)$$

$$2\rho E = \int \xi^2 f d\boldsymbol{\xi} \quad (2.30c)$$

with integrals computed over \mathbb{R} . Hereafter, integration bounds will be omitted for the sake of clarity.

Regarding the collision model Ω_f , it must satisfy the conservation of mass, momentum and total energy:

$$\int \Omega_f \Phi(\boldsymbol{\xi}) d\boldsymbol{\xi} = 0 \quad (2.31)$$

with $\Phi(\boldsymbol{\xi}) = (1, \boldsymbol{\xi}, \xi^2/2)$, and note that $\xi^2 = \boldsymbol{\xi} \cdot \boldsymbol{\xi} = |\boldsymbol{\xi}|^2$.

Most common collision models are based on linearized ones, such as the single relaxation time (SRT) collision term of Bhatnagar-Gross-Krook (BGK). The BGK single-relaxation-time collision model Ω_f^{BGK} is:

$$\Omega_f^{\text{BGK}} = -\frac{1}{\tau}(f - f^{\text{eq}}) \quad (2.32)$$

where τ is the relaxation time of collisions to equilibrium, f^{eq} represents a local equilibrium distribution (i.e. Maxwell-Boltzmann, or called Maxwellian) in the reference frame moving with the bulk of the flow, as shown in Eq. (2.21). From discussions in Section 2.1.2 and Section 2.1.3, Eq. (2.31) can be met.

2.1.5 Non-dimensionalization

2.1.5.1 Non-dimensional Boltzmann Equation

We now derive the non-dimensional, continuous Boltzmann equation.

For a fluid, if its characteristic length l_o and characteristic velocity v_o are determined, the characteristic time scale is then given by $t_o = l_o/v_o$.

We use superscript “*” to denote dimensionless quantities, and use subscript “o” to denote characteristic quantities with physical units. We first introduce the dimensionless derivatives:

$$\left. \begin{aligned} \frac{\partial}{\partial t^*} &= \frac{l_o}{v_o} \frac{\partial}{\partial t} \\ \frac{\partial}{\partial x^*} &= l_o \frac{\partial}{\partial x} \\ \frac{\partial}{\partial \xi^*} &= v_o \frac{\partial}{\partial \xi} \end{aligned} \right\} \Rightarrow \left\{ \begin{aligned} \frac{\partial}{\partial t} &= \frac{v_o}{l_o} \frac{\partial}{\partial t^*} \\ \frac{\partial}{\partial x} &= \frac{1}{l_o} \frac{\partial}{\partial x^*} \\ \frac{\partial}{\partial \xi} &= \frac{1}{v_o} \frac{\partial}{\partial \xi^*} \end{aligned} \right. \quad (2.33)$$

Substitute the dimensionless derivatives into the continuous Boltzmann equation shown in Eq. (2.29), and note that the velocity $\xi_\alpha = v_o \xi_\alpha^*$ and the acceleration $g_\alpha = \frac{v_o^2}{l_o} g_\alpha^*$, therefore

$$\frac{v_o}{l_o} \frac{\partial f}{\partial t^*} + v_o \xi_\alpha^* \frac{1}{l_o} \frac{\partial f}{\partial x^*} + \frac{v_o^2}{l_o} g_\alpha^* \frac{1}{v_o} \frac{\partial f}{\partial \xi^*} = \Omega(f) \quad (2.34)$$

As introduced, in D -dimensional space, the dimension $[f] = [\rho]/[v^D]$, we define the dimensionless mass density distribution function

$$f^* = \frac{f v_o^D}{\rho_o}$$

where ρ_o is the density (with physical unit) calculated with characteristic quantities.

For the collision operator $\Omega(f) = -\frac{1}{\tau}(f - f^{\text{eq}})$, the equilibrium distribution function shown in Eq. (2.21) can also be non-dimensionalized as shown in Eq. (2.41) with $f^{\text{eq}*} = \frac{f^{\text{eq}} v_o^D}{\rho_o}$, thus we can denote the non-dimensionalized form of the collision operator $\Omega(f) = -\frac{1}{\tau}(f - f^{\text{eq}})$ as $\Omega(f^*) = -\frac{1}{\tau}(f^* - f^{\text{eq}*})$, and since the distribution functions f or f^{eq} appears in every term of the continuous Boltzmann equation shown in Eq. (2.29), and τ is dimensionless, as discussed in discrete Boltzmann Equation shown in Eq. (4.9), the introduced scaling variables v_o^D and ρ_o will be canceled at both sides. Thus we can final obtain the non-dimensional Boltzmann equation

$$\frac{\partial f}{\partial t^*} + \xi_\alpha^* \frac{\partial f}{\partial x^*} + g_\alpha^* \frac{\partial f}{\partial \xi^*} = \Omega(f^*) \quad (2.35)$$

which has the same form of the dimensional Boltzmann equation as shown in Eq. (2.29), thus Eq. (2.29) can be seen as either a dimensional form or a non-dimensional form.

2.1.5.2 Non-dimensional Equilibrium Distribution Function

Now we derive the dimensionless form of the Maxwellian for f^{eq} .

First, recognize the Boltzmann constant k defined in Definition 1.3.3 has a unit of $\text{J} \cdot \text{K}^{-1}$, or for the Maxwellian in Eq. (2.21), the dimension $[kT] = [mc^2] = \text{J}$ is a dimension of energy. Thus, the Maxwellian has a dimension of $[f^{\text{eq}}] = [\rho]/[c^D] = \frac{\text{kg}}{\text{m}^3} \times \frac{1}{(\text{m/s})^D}$.

Maxwellian can be non-dimensionalized through selection of appropriate scales as follows:

Quantities with a superscript “*” are dimensionless quantities and quantities with a subscript “o”

Table 2.1: Enter table caption here.

scale	dimensionless variable
length	$l^* = x/l_o$
velocity	$c^* = c/c_o$
time	$t^* = t/t_o = tc_o/l_o$
molecule mass	$m^* = m/m_o$
density	$\rho^* = \rho/\rho_o$
temperature	$T^* = T/T_o$
Boltzmann constant	$k^* = k/k_o$

are characteristic quantities with physical units.

Thus the Maxwellian in Eq. (2.21) will become

$$\begin{aligned}
 f^{\text{eq}} &= \rho \left(\frac{m}{2\pi kT} \right)^{D/2} \exp \left(-\frac{mc^2}{2kT} \right) \\
 &= \rho^* \rho_o \left(\frac{m^* m_o}{2\pi k^* k_o T^* T_o} \right)^{D/2} \exp \left(-\frac{m^* m_o c^{*2} c_o^2}{2k^* k_o T^* T_o} \right)
 \end{aligned}$$

The characteristic quantities can be choosing to be any value as long as the relevant ones are correlated, such as if the characteristic length l_o and characteristic velocity c_o are determined, the characteristic time scale is then given by $t_o = l_o/c_o$. Thus, for convenience, since $[kT] = [mc^2] = \text{J}$, we choose the characteristic velocity to be $c_o \equiv \sqrt{k_o T_o / m_o}$ as by Shan et al. [5]. Refer to Eq. (1.126), c_o is easily recognized as the *sound speed* at temperature T_o . Thus

$$f^{\text{eq}} = \left(\frac{\rho^* \rho_o}{c_o^D} \right) \left(\frac{m^*}{2\pi k^* T^*} \right)^{D/2} \exp \left(-\frac{m^* c^{*2}}{2k^* T^*} \right)$$

Since the dimension $[f^{\text{eq}}] = [\rho]/[c^D]$, we define the dimensionless Maxwellian as

$$f^{\text{eq}*} = \frac{f^{\text{eq}} c_o^D}{\rho_o}$$

Therefore,

$$f^{\text{eq}*} = \rho^* \left(\frac{m^*}{2\pi k^* T^*} \right)^{D/2} \exp \left(-\frac{m^* c^{*2}}{2k^* T^*} \right) \quad (2.36)$$

We can see that the dimensionless Maxwellian remain the same form as the Maxwellian with dimensions shown in Eq. (2.21). We now consider ideal gas law under this dimensionless framework.

Now we define another dimensionless variable $\theta^* = \frac{k^* T^*}{m^*}$, which is dimensionless temperature by Shan et al. [6]. However, a careful examination of this variable θ^* show that it is a dimensionless variable stems from $\theta = \frac{kT}{m}$ which has a unit of $[c^2] = \text{m}^2 \cdot \text{sec}^{-2}$. So that's why usually we will see the lattice temperature is $1/3$ which is also equivalent to the squared sound speed in LBM. So we can update the Maxwellian the get a simplified version:

$$f^{\text{eq}*} = \frac{\rho^*}{(2\pi\theta^*)^{D/2}} \exp \left(-\frac{c^{*2}}{2\theta^*} \right) \quad (2.37)$$

From the ideal gas law, $p = \rho \frac{R}{M} T = \rho \frac{k}{m} T$ shown in Eq. (1.78), we have

$$p = \rho \frac{k}{m} T = \frac{\rho^* \rho_o k^* k_o T^* T_o}{m^* m_o} = \frac{\rho^* k^* T^*}{m^*} \rho_o c_o^2 \quad (2.38)$$

Since $[p] = [\rho c^2] = \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-2}$ (Section 1.3.5.4), we define the dimensionless pressure as

$$p^* = \frac{p}{\rho_o c_o^2} \quad (2.39)$$

The ideal gas law following the same form:

$$p^* = \frac{\rho^* k^* T^*}{m^*} = \rho^* \theta^* \quad (2.40)$$

In discussions hereafter, the dimensionless variables are used unless otherwise specified. So the simplified dimensionless Maxwellian can be written without using the asterisk superscript, as

$$f^{\text{eq}} = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left(-\frac{c^2}{2\theta}\right) = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left(-\frac{|\boldsymbol{\xi} - \mathbf{u}|^2}{2\theta}\right) \quad (2.41)$$

Note that $c^2 = \mathbf{c} \cdot \mathbf{c} = |\mathbf{c}|^2$, and $|\boldsymbol{\xi} - \mathbf{u}|^2 = (\boldsymbol{\xi} - \mathbf{u}) \cdot (\boldsymbol{\xi} - \mathbf{u})$, all involve scalar product, both are the magnitude of the intrinsic velocity \mathbf{c} , as shown in Eq. (2.12). Hereinafter, velocities $\boldsymbol{\xi}$, \mathbf{u} and \mathbf{c} are to be understood as dimensionless measured in the units of characteristic velocity c_o , and all velocity moments defined in Eq. (2.2), Eq. (2.7), Eq. (2.9), and Eq. (2.11). Thus, the mass density ρ , the dimensionless fluid velocity \mathbf{u} , and the dimensionless internal energy⁴ will be $e = \frac{D}{2} \frac{RT}{M} = \frac{D}{2} \frac{kT}{m} = \frac{D}{2} \theta$ as discussed in Section 2.1.2, are expressed as the velocity moments of the form $\int f \varphi(\boldsymbol{\xi}) d\boldsymbol{\xi}$, with $\varphi = 1$, $\boldsymbol{\xi}$, and ξ^2 , respectively [7]:

$$\rho = \int f d\boldsymbol{\xi} \quad (2.42a)$$

$$\rho \mathbf{u} = \int \boldsymbol{\xi} f d\boldsymbol{\xi} \quad (2.42b)$$

$$2\rho E = 2\rho e + \rho u^2 = \int \xi^2 f d\boldsymbol{\xi} \quad (2.42c)$$

Note that the squared velocity magnitude $u^2 = \mathbf{u} \cdot \mathbf{u} = |\mathbf{u}|^2$ and $\xi^2 = \boldsymbol{\xi} \cdot \boldsymbol{\xi} = |\boldsymbol{\xi}|^2$ involve dot product. Of course, at constant temperature $\theta = 1$, the sound speed in the gas system is unity, refer to Eq. (1.124) and for isothermal process.

2.2 Lattice Boltzmann Dynamics

2.2.1 Discrete Equilibrium Distribution Function

The equilibrium distribution function $f_i^{\text{eq}}(\mathbf{r}, t)$ reads [4, 8, 9, 10] (need a derivation why feq has such form based on the Chapman-Enskog Expansion, refer to [11]):

⁴Here, the internal energy with unit mass is actually referred

$$f_i^{\text{eq}} = w_i \rho \left\{ 1 + \frac{\mathbf{c}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{c}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2} \right\} \quad (2.43a)$$

$$= w_i \rho \left(1 + \frac{1}{c_s^2} \mathbf{c}_i \cdot \mathbf{u} + \frac{1}{2c_s^4} \mathbf{Q}_i : \mathbf{u} \mathbf{u} \right) \quad (2.43b)$$

$$= w_i \rho \left(1 + \frac{1}{c_s^2} c_{i\alpha} u_\alpha + \frac{1}{2c_s^4} Q_{i\alpha\beta} u_\alpha u_\beta \right) \quad (2.43c)$$

$$= w_i \rho \left\{ 1 + \frac{c_{i\alpha} u_\alpha}{c_s^2} + \frac{u_\alpha u_\beta (c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta})}{2c_s^4} \right\} \quad (2.43d)$$

where $\mathbf{Q}_i = \mathbf{c}_i \mathbf{c}_i - c_s^2 \mathbf{I}$, or $Q_{i\alpha\beta} = c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta}$, in which \mathbf{I} is the identity matrix (or sometimes ambiguously called a unit matrix) and $\delta_{\alpha\beta}$ is the Kronecker delta. The lattice sound speed $c_s = \frac{c}{\sqrt{3}}$, and in which the lattice speed $c = \delta_h / \delta_t = 1$ for a standard square lattice with the lattice spacing $\delta_h = \delta_x = \delta_y = 1$ and thus the lattice time step $\delta_t = 1$.

The double dot product [12, 13] in Eq. (2.43) can be defined as⁵: $\mathbf{A} : \mathbf{B} = A_{ij} B_{ij}$, thus

$$\mathbf{Q}_i : \mathbf{u} \mathbf{u} = (\mathbf{c}_i \mathbf{c}_i - c_s^2 \mathbf{I}) : \mathbf{u} \mathbf{u} \quad (2.44a)$$

$$= \begin{bmatrix} c_{i\alpha} c_{i\alpha} & c_{i\alpha} c_{i\beta} \\ c_{i\beta} c_{i\alpha} & c_{i\beta} c_{i\beta} \end{bmatrix} : \begin{bmatrix} u_\alpha u_\alpha & u_\alpha u_\beta \\ u_\beta u_\alpha & u_\beta u_\beta \end{bmatrix} - c_s^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} : \begin{bmatrix} u_\alpha u_\alpha & u_\alpha u_\beta \\ u_\beta u_\alpha & u_\beta u_\beta \end{bmatrix} \quad (2.44b)$$

$$= (c_{i\alpha}^2 u_\alpha^2 + 2c_{i\alpha} c_{i\beta} u_\alpha u_\beta + c_{i\beta}^2 u_\beta^2) - c_s^2 (u_\alpha u_\alpha + u_\beta u_\beta) \quad (2.44c)$$

$$= (c_{i\alpha} u_\alpha + c_{i\beta} u_\beta)^2 - c_s^2 \mathbf{u} \cdot \mathbf{u} \quad (2.44d)$$

$$= (\mathbf{c}_i \cdot \mathbf{u})^2 - c_s^2 \mathbf{u} \cdot \mathbf{u} \quad (2.44e)$$

This means that the equilibrium distribution functions defined with different forms in Eq. (2.43) are equivalent. As discussed, the tensor product of the velocity vector $\mathbf{u} \mathbf{u}$ should follow:

$$\mathbf{u} \mathbf{u} = \mathbf{u} \otimes \mathbf{u} = \mathbf{u} \mathbf{u}^T = \begin{bmatrix} u_\alpha \\ u_\beta \end{bmatrix} \begin{bmatrix} u_\alpha & u_\beta \end{bmatrix} = \begin{bmatrix} u_\alpha u_\alpha & u_\alpha u_\beta \\ u_\beta u_\alpha & u_\beta u_\beta \end{bmatrix} \quad (2.45)$$

2.2.2 Various Forms BGK Dynamics

With the understanding of the equilibrium and non-equilibrium distribution functions, we can summarize a various forms of the collision and streaming (advection) process of the Boltzmann-BGK equation as:

⁵There are two double dot product definitions, both are fine here.

$$f_i(\mathbf{r} + \mathbf{c}_i \delta_t, t + \delta_t) = f_i(\mathbf{r}, t) - \frac{1}{\tau} \{f_i(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r}, t)\} \quad (2.46a)$$

$$= f_i(\mathbf{r}, t) - \omega \{f_i(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r}, t)\} \quad (2.46b)$$

$$= (1 - \omega)f_i(\mathbf{r}, t) + \omega f_i^{\text{neq}}(\mathbf{r}, t) \quad (2.46c)$$

$$= f_i(\mathbf{r}, t) - \omega f_i^{\text{neq}}(\mathbf{r}, t) \quad (2.46d)$$

$$= \{f_i^{\text{eq}}(\mathbf{r}, t) + f_i^{\text{neq}}(\mathbf{r}, t)\} - \omega f_i^{\text{neq}}(\mathbf{r}, t) \quad (2.46e)$$

$$= f_i^{\text{eq}}(\mathbf{r}, t) + (1 - \omega)f_i^{\text{neq}}(\mathbf{r}, t) \quad (2.46f)$$

where $\omega = \frac{1}{\tau}$ is called the relaxation frequency.

Whichever the BGK dynamics form, the Boltzmann-BGK equation can be solved in two steps:

$$\begin{cases} f_i^*(\mathbf{r}, t) = f_i(\mathbf{r}, t) - \frac{1}{\tau} \{f_i(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r}, t)\} & \text{(Collision)} \\ f_i(\mathbf{r} + \mathbf{c}_i \delta_t, t + \delta_t) = f_i^*(\mathbf{r}, t) & \text{(Streaming)} \end{cases} \quad (2.47)$$

As derived in Eq. (4.73), the relaxation time relates the lattice kinematic viscosity as $\nu = \frac{\tau - 1/2}{3}$. Thus, as discussed by Li [14], when τ is close to 0.5, fluid viscosity is small, in other words, particle distribution may become negative ($f_i(\mathbf{r}, t) < 0$). To suppress the negative distributions and improve numerical stability, a protection procedure of positivity for distributions can be applied, consider the following procedure after collision:

$$\begin{aligned} f_i(\mathbf{r}, t) - \frac{1}{\tau} \{f_i(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r}, t)\} &> 0 \\ \left(1 - \frac{1}{\tau}\right) f_i(\mathbf{r}, t) + \frac{1}{\tau} f_i^{\text{eq}}(\mathbf{r}, t) &> 0 \\ (\tau - 1) f_i(\mathbf{r}, t) + f_i^{\text{eq}}(\mathbf{r}, t) &> 0 \\ \tau &> 1 - \frac{f_i^{\text{eq}}(\mathbf{r}, t)}{f_i(\mathbf{r}, t)} \end{aligned}$$

The above procedure assumes $\tau > 0$. Thus, a new local relaxation time can be defined as:

$$\tilde{\tau}(\mathbf{r}, t) = \max \left\{ \tau, 1 - \frac{f_i^{\text{eq}}(\mathbf{r}, t)}{f_i(\mathbf{r}, t)} \right\} \quad (2.48)$$

Through this procedure, a positive distribution is guaranteed after each collision as long as it is positive before the collision. In other words, by effectively adding a local viscosity lower bound, which is dynamically local distribution dependent, we are able to keep distributions positive and improve the simulation stability [14].

2.2.3 Macroscopic Moments

Using the general equilibrium distribution in Eq. (2.43) together with the isotropy conditions based on Hermite polynomials, we can find the equilibrium moments explicitly:

$$\Gamma^{\text{eq}} = \sum_i f_i^{\text{eq}} = \rho \quad (2.49a)$$

$$\Gamma_{\alpha}^{\text{eq}} = \sum_i c_{i\alpha} f_i^{\text{eq}} = \rho u_{\alpha} \quad (2.49b)$$

$$\Gamma_{\alpha\beta}^{\text{eq}} = \sum_i c_{i\alpha} c_{i\beta} f_i^{\text{eq}} = c_s^2 \rho \delta_{\alpha\beta} + \rho u_{\alpha} u_{\beta} \quad (2.49c)$$

$$\Gamma_{\alpha\beta\gamma}^{\text{eq}} = \sum_i c_{i\alpha} c_{i\beta} c_{i\gamma} f_i^{\text{eq}} = c_s^2 \rho (u_{\alpha} \delta_{\beta\gamma} + u_{\beta} \delta_{\alpha\gamma} + u_{\gamma} \delta_{\alpha\beta}) \quad (2.49d)$$

We will prove it that the equation of state for the LBE is $p = c_s^2 \rho$. This part has been discussed in Section 1.3.5.4 and Section 2.1.5.

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Chapter 3 The Discrete Hermite Transform

3.1 Hermite Polynomials

In mathematics, the Hermite polynomials are a classical orthogonal polynomial sequence.¹

The mathematical property of the Hermite polynomials, especially that in higher dimensions, has been extensively treated by Grad [1]. As demonstrated below, a unique feature in using the Hermite polynomials as the expansion basis rather than any other functions is that the expansion coefficients correspond precisely to the velocity moments up to the given degrees.

3.1.1 Definition and Properties of Hermite Polynomials

3.1.1.1 Definition

The Hermite polynomials are orthogonal on the interval $(-\infty, \infty)$ with respect to the normal distribution (or called the weight function).

$$\omega(x) = e^{-\frac{x^2}{2}}, \text{ or} \quad (3.1)$$

$$\omega(x) = e^{-x^2} \quad (3.2)$$

Definition 3.1.1 – Hermite polynomials. There are two different ways of standardizing the Hermite polynomials, which can be expressed by Rodrigues formula [2, 3]:

- The Hermite polynomials for probabilists are given by

$$He_n(x) = \frac{(-1)^n}{\omega(x)} D^n \omega(x) = (-1)^n e^{\frac{x^2}{2}} D^n e^{-\frac{x^2}{2}} = (-1)^n e^{\frac{x^2}{2}} \frac{d^n}{dx^n} e^{-\frac{x^2}{2}}, \quad n = 0, 1, 2, \dots \quad (3.3)$$

- The Hermite polynomials for physicists are given by

$$H_n(x) = \frac{(-1)^n}{\omega(x)} D^n \omega(x) = (-1)^n e^{x^2} D^n e^{-x^2} = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \quad n = 0, 1, 2, \dots \quad (3.4)$$

where the differentiation operator D is defined by $D = \frac{d}{dx}$, thus $D^n = \left(\frac{d}{dx}\right)^n = \frac{d^n}{(dx)^n}$, and here we use the short notation $D^n = \frac{d^n}{(dx)^n} = \frac{d^n}{dx^n}$. Also, the definition of Hermite polynomials implies that $He_0(x) = 1$ and $H_0(x) = 1$.

Hermite polynomials are standardized in two different ways depending on their use, they are: the Chebyshev-Hermite polynomials, $\{He_n(x)\}_{n=0}^{\infty}$ (regularly applied in probability) and the Hermite polynomials, $\{H_n(x)\}_{n=0}^{\infty}$ (frequently applied in physics).

Sometimes the naming of the polynomials change from author to author, however the mathematical notation for both is currently well distinct in the technical literature. They both share

¹In mathematics, a polynomial sequence is a sequence of polynomials indexed by the nonnegative integers 0, 1, 2, 3, ... in which each index is equal to the degree of the corresponding polynomial. Polynomial sequences are a topic of interest in enumerative combinatorics and algebraic combinatorics, as well as applied mathematics.

the following relationship [2, 4],

$$H_n(x) = 2^{\frac{n}{2}} He_n(\sqrt{2}x) \quad (3.5a)$$

$$He_n(x) = 2^{-\frac{n}{2}} H_n\left(\frac{x}{\sqrt{2}}\right) \quad (3.5b)$$

The polynomials He_n are sometimes denoted by H_n , especially in probability theory, because $\frac{1}{\sqrt{2\pi}}e^{-\frac{1}{2}x^2}$ is the probability density function for the normal distribution with expected value 0 and standard deviation 1, which is the simplest case of a normal distribution, also known as the standard normal distribution.

The first six probabilists' Hermite polynomials are:

$$He_0(x) = 1 \quad (3.6a)$$

$$He_1(x) = x \quad (3.6b)$$

$$He_2(x) = x^2 - 1 \quad (3.6c)$$

$$He_3(x) = x^3 - 3x \quad (3.6d)$$

$$He_4(x) = x^4 - 6x^2 + 3 \quad (3.6e)$$

$$He_5(x) = x^5 - 10x^3 + 15x \quad (3.6f)$$

The first six physicists' Hermite polynomials are:

$$H_0(x) = 1 \quad (3.7a)$$

$$H_1(x) = 2x \quad (3.7b)$$

$$H_2(x) = 4x^2 - 2 \quad (3.7c)$$

$$H_3(x) = 8x^3 - 12x \quad (3.7d)$$

$$H_4(x) = 16x^4 - 48x^2 + 12 \quad (3.7e)$$

$$H_5(x) = 32x^5 - 160x^3 + 120x \quad (3.7f)$$

The n th-order Hermite polynomial $He_n(x)$ or $H_n(x)$ is a polynomial of degree n . Further we have that $He_{2n}(x)$ or $H_{2n}(x)$ is even, and $He_{2n+1}(x)$ or $H_{2n+1}(x)$ is odd. The probabilists' version $He_n(x)$ has leading coefficient of $k_n = 1$, while the physicists' version $H_n(x)$ has leading coefficient of $k_n = 2^n$.

The first six physicists' Hermite polynomials $H_n(x)$ are plotted, as shown in Fig 3.1. Note that the Hermite polynomials are scaled down by a factor of n^2 in order to be fit on the same plot.

3.1.1.2 Derivation of Properties of the Hermite Polynomials

First, we derive the orthogonality of the Hermite polynomials.

Definition 3.1.2 – Orthogonal polynomials. A sequence of polynomials $\{p_n(x)\}_{n=0}^{\infty}$, where n is the degree of $p_n(x)$, i.e. $\text{degree}[p_n(x)] = n$, is said to be a sequence of **orthogonal** polynomials (or called orthogonal) with respect to the weight function $\omega(x)$ on the interval (a, b) with $a < b$

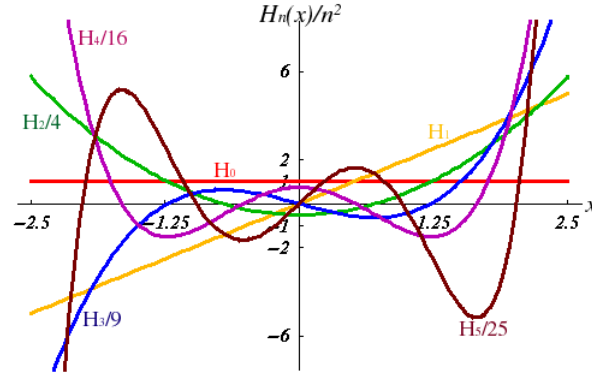


Figure 3.1: The First Six Hermite Polynomials $H_n(x)/n^2$

if

$$\int_a^b \omega(x) p_m(x) p_n(x) dx = h_n \delta_{nm} \quad \text{with} \quad \delta_{nm} := \begin{cases} 0, & \text{if } m \neq n \\ 1, & \text{if } m = n \end{cases} \quad (3.8)$$

where h_n are given constants and δ_{nm} is the Kronecker delta. The weight function $\omega(x)$ should be continuous and positive on (a, b) such that the moments

$$\mu_m := \int_a^b \omega(x) x^m dx, \quad m = 0, 1, 2, \dots \quad (3.9)$$

exist. Then the integral

$$\langle f, g \rangle := \int_a^b \omega(x) f(x) g(x) dx \quad (3.10)$$

denotes an inner product of the polynomials f and g . The interval (a, b) is called the interval of orthogonality. This interval can be infinite over the interval \mathbb{R} .

If $h_n = 1$ for each $n \in \{0, 1, 2, \dots\}$ the sequence of polynomials is called **orthonormal**.

The Hermite polynomials satisfy the orthogonality relation

$$\begin{aligned} \int_{-\infty}^{\infty} e^{-x^2/2} H_m(x) H_n(x) dx &= \sqrt{2\pi} n! \delta_{nm}, \quad m, n \in \{0, 1, 2, \dots\} \\ \int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx &= \sqrt{\pi} 2^n n! \delta_{nm}, \quad m, n \in \{0, 1, 2, \dots\} \end{aligned}$$

To prove this we use the definition in Eq. (3.4) to obtain

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx = (-1)^n \int_{-\infty}^{\infty} H_m(x) D^n e^{-x^2} dx \quad (3.11)$$

Now we use integration by parts n times to conclude that the integral vanishes for $m < n$. This is because $H_m(x)$ has a polynomial degree of m (refer to the examples of the first six Hermite polynomials), and through the integration by parts n times, the integral will vanish, this will be clear in the following situation with $m = n$.

For $m = n$ we have using integration by parts refer to Theorem 1.3.1, and consider the Gaussian

integrals in Section 1.3.2 that $\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$, for $H_n(x)$ we have:

$$\begin{aligned}
 \int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx &= (-1)^n \int_{-\infty}^{\infty} H_n(x) D^n e^{-x^2} dx \\
 &= (-1)^n \int_{-\infty}^{\infty} H_n(x) D(D^{n-1} e^{-x^2}) dx \\
 &= (-1)^n \left\{ H_n(x) D^{n-1} e^{-x^2} \right\}_{-\infty}^{\infty} - (-1)^n \int_{-\infty}^{\infty} \{DH_n(x)\} (D^{n-1} e^{-x^2}) dx \\
 &= 0 + (-1)^{n+1} \int_{-\infty}^{\infty} \{DH_n(x)\} D(D^{n-2} e^{-x^2}) dx \\
 &= 0 + (-1)^{n+2} \int_{-\infty}^{\infty} \{D^2 H_n(x)\} (D^{n-2} e^{-x^2}) dx \\
 &= 0 + (-1)^{2n} \int_{-\infty}^{\infty} \{D^n H_n(x)\} (D^0 e^{-x^2}) dx \\
 &= k_n n! \int_{-\infty}^{\infty} e^{-x^2} dx \\
 &= \sqrt{\pi} 2^n n!
 \end{aligned}$$

The value of $\left\{ H_n(x) D^{n-1} e^{-x^2} \right\}_{-\infty}^{\infty}$ equals 0 for both ends, this is because of the L'Hospital's rule in Theorem 1.3.2.

Same procedures can be applied to $He_n(x)$ for $m = n$, we have

$$\begin{aligned}
 \int_{-\infty}^{\infty} e^{-x^2/2} He_m(x) He_n(x) dx &= (-1)^n \int_{-\infty}^{\infty} He_n(x) D^n e^{-x^2/2} dx \\
 &= k_n n! \int_{-\infty}^{\infty} e^{-x^2/2} dx \\
 &= \sqrt{2\pi} n!
 \end{aligned}$$

Remember that for $He_n(x)$, the leading coefficient $k_n = 1$; while for $H_n(x)$ the leading coefficient $k_n = 2^n$.

Second, we derive the recurrence relation of the Hermite polynomials.

Since $D^{n+1} = DD^n$, refer to Eq. (3.3) and Eq. (3.4), we have $D^n \omega(x) = (-1)^n \omega(x) He_n(x)$ and $D^n \omega(x) = (-1)^n \omega(x) H_n(x)$. Also, for the weight functions we have

$$\omega(x) = e^{-x^2/2} \implies \omega'(x) = -x\omega(x) \quad (3.12a)$$

$$\omega(x) = e^{-x^2} \implies \omega'(x) = -2x\omega(x) \quad (3.12b)$$

For $He_n(x)$ we obtain

$$\begin{aligned}
D^{n+1}\omega(x) &= D\{D^n\omega(x)\} \\
&= (-1)^n D\{\omega(x)He_n(x)\} \\
&= (-1)^n \{\omega'(x)He_n(x) + \omega(x)He'_n(x)\} \\
&= (-1)^n \{-x\omega(x)He_n(x) + \omega(x)He'_n(x)\} \\
&= (-1)^{n+1}\omega(x)\{xHe_n(x) - He'_n(x)\}, \quad n = 0, 1, 2, \dots
\end{aligned}$$

which implies that (by considering $He_{n+1}(x) = \frac{(-1)^{n+1}}{\omega(x)} D^{n+1}\omega(x)$)

$$\boxed{He_{n+1}(x) = xHe_n(x) - He'_n(x)}, \quad n = 0, 1, 2, \dots \quad (3.13)$$

Or for $H_n(x)$ we obtain

$$\begin{aligned}
D^{n+1}\omega(x) &= D\{D^n\omega(x)\} \\
&= (-1)^n D\{\omega(x)H_n(x)\} \\
&= (-1)^n \{\omega'(x)H_n(x) + \omega(x)H'_n(x)\} \\
&= (-1)^n \{-2x\omega(x)H_n(x) + \omega(x)H'_n(x)\} \\
&= (-1)^{n+1}\omega(x)\{2xH_n(x) - H'_n(x)\}, \quad n = 0, 1, 2, \dots
\end{aligned}$$

which implies that (by considering $H_{n+1}(x) = \frac{(-1)^{n+1}}{\omega(x)} D^{n+1}\omega(x)$)

$$\boxed{H_{n+1}(x) = 2xH_n(x) - H'_n(x)}, \quad n = 0, 1, 2, \dots \quad (3.14)$$

In order to find the three term recurrence relation we introduce the general Leibniz rule [5]:

Theorem 3.1.1 – General Leibniz rule. In calculus, the general Leibniz rule, named after Gottfried Wilhelm Leibniz, generalizes the product rule (which is also known as “Leibniz’s rule”). It states that if f and g are n -times differentiable functions, then the product fg is also n -times differentiable and its n th derivative is given by

$$(fg)^{(n)} = \sum_{k=0}^n \binom{n}{k} f^{(n-k)} g^{(k)} \quad (3.15)$$

where $\binom{n}{k} = \frac{n!}{k!(n-k)!}$ is the binomial coefficient and $f^{(0)} \equiv f$.

Proof: The proof of the general Leibniz rule proceeds by induction. Let f and g be n -times differentiable functions. The base case when $n = 1$ claims that:

$$(fg)' = f'g + fg'$$

which is the usual product rule and is known to be true. Next, assume that the statement holds for a fixed $n \geq 1$ that is, that

$$(fg)^{(n)} = \sum_{k=0}^n \binom{n}{k} f^{(n-k)} g^{(k)}$$

Then,

$$\begin{aligned}
 (fg)^{(n+1)} &= \left\{ \sum_{k=0}^n \binom{n}{k} f^{(n-k)} g^{(k)} \right\}' \\
 &= \sum_{k=0}^n \binom{n}{k} f^{(n+1-k)} g^{(k)} + \sum_{k=0}^n \binom{n}{k} f^{(n-k)} g^{(k+1)} \\
 &= \sum_{k=0}^n \binom{n}{k} f^{(n+1-k)} g^{(k)} + \sum_{k=1}^{n+1} \binom{n}{k-1} f^{(n+1-k)} g^{(k)} \\
 &= \binom{n}{0} f^{(n+1)} g + \sum_{k=1}^n \binom{n}{k} f^{(n+1-k)} g^{(k)} + \sum_{k=1}^n \binom{n}{k-1} f^{(n+1-k)} g^{(k)} + \binom{n}{n} f g^{(n+1)} \\
 &= f^{(n+1)} g + \left\{ \sum_{k=1}^n \left[\binom{n}{k-1} + \binom{n}{k} \right] f^{(n+1-k)} g^{(k)} \right\} + f g^{(n+1)} \\
 &= f^{(n+1)} g + \sum_{k=1}^n \binom{n+1}{k} f^{(n+1-k)} g^{(k)} + f g^{(n+1)} \\
 &= \sum_{k=0}^{n+1} \binom{n+1}{k} f^{(n+1-k)} g^{(k)}
 \end{aligned}$$

And so the statement holds for $n + 1$ and the proof is complete.

Note that in the derivation process,

$$\begin{aligned}
 \binom{n}{k-1} + \binom{n}{k} &= \frac{n!}{(k-1)!(n-k+1)!} + \frac{n!}{k!(n-k)!} \\
 &= \frac{n!k}{k!(n-k+1)!} + \frac{n!(n-k+1)}{k!(n-k+1)!} \\
 &= \frac{n!(n+1)}{k!(n+1-k)!} \\
 &= \frac{(n+1)!}{k!(n+1-k)!} \\
 &= \binom{n+1}{k}
 \end{aligned}$$

Definition 3.1.3 – Binomial coefficient. In mathematics, the binomial coefficients are the positive integers that occur as coefficients in the binomial theorem. Commonly, a binomial coefficient is indexed by a pair of integers $n \geq k \geq 0$ and is written $\binom{n}{k}$. It is the coefficient of the x^k term in the polynomial expansion of the binomial power $(1+x)^n$, and it is given by the formula

$$\binom{n}{k} = \frac{n!}{k!(n-k)!} \quad (3.16)$$

The binomial coefficient satisfies the following recurrence relation [6]:

$$\binom{n}{k} = \binom{n-1}{k} + \binom{n-1}{k-1} \quad (3.17)$$

This is because

$$\begin{aligned} \binom{n-1}{k} + \binom{n-1}{k-1} &= \frac{(n-1)!}{k!(n-1-k)!} + \frac{(n-1)!}{(k-1)!(n-k)!} \\ &= \frac{(n-1)!(n-k)}{k!(n-k)!} + \frac{(n-1)!k}{k!(n-k)!} \\ &= \frac{(n-1)!n}{k!(n-k)!} \\ &= \frac{n!}{k!(n-k)!} \\ &= \binom{n}{k} \end{aligned}$$

We come back to the Hermite polynomials and use the general Leibniz rule.

For $He_n(x)$ we obtain

$$\begin{aligned} D^{n+1}\omega(x) &= D^n\omega'(x) \\ &= D^n\{-x\omega(x)\} \\ &= -\left\{\sum_{k=0}^n \binom{n}{k} x^{(n-k)} \omega^{(k)}(x)\right\} \\ &= -\left\{\binom{n}{n} x^{(0)} \omega^{(n)}(x) + \binom{n}{n-1} x^{(1)} \omega^{(n-1)}(x) + 0 + \dots + 0\right\} \\ &= -x\omega^{(n)}(x) - n\omega^{(n-1)}(x) \\ &= -xD^n\omega(x) - nD^{n-1}\omega(x) \end{aligned}$$

by considering $He_{n+1}(x) = \frac{(-1)^{n+1}}{\omega(x)} D^{n+1}\omega(x)$, we have

$$\begin{aligned} \frac{(-1)^{n+1}}{\omega(x)} D^{n+1}\omega(x) &= -x \frac{(-1)^{n+1}}{\omega(x)} D^n\omega(x) - n \frac{(-1)^{n+1}}{\omega(x)} D^{n-1}\omega(x) \\ &= x \frac{(-1)^n}{\omega(x)} D^n\omega(x) - n \frac{(-1)^{n-1}}{\omega(x)} D^{n-1}\omega(x) \end{aligned}$$

which implies that

$$\boxed{He_{n+1}(x) = xHe_n(x) - nHe_{n-1}(x)}, \quad n = 0, 1, 2, \dots \quad (3.18)$$

For $H_n(x)$ we obtain

$$\begin{aligned}
D^{n+1}\omega(x) &= D^n\omega'(x) \\
&= D^n\{-2x\omega(x)\} \\
&= -2\left\{\sum_{k=0}^n \binom{n}{k} x^{(n-k)}\omega^{(k)}(x)\right\} \\
&= -2\left\{\binom{n}{n}x^{(0)}\omega^{(n)}(x) + \binom{n}{n-1}x^{(1)}\omega^{(n-1)}(x) + 0 + \cdots + 0\right\} \\
&= -2x\omega^{(n)}(x) - 2n\omega^{(n-1)}(x) \\
&= -2xD^n\omega(x) - 2nD^{n-1}\omega(x)
\end{aligned}$$

by considering $H_{n+1}(x) = \frac{(-1)^{n+1}}{\omega(x)}D^{n+1}\omega(x)$, we have

$$\begin{aligned}
\frac{(-1)^{n+1}}{\omega(x)}D^{n+1}\omega(x) &= -2x\frac{(-1)^{n+1}}{\omega(x)}D^n\omega(x) - 2n\frac{(-1)^{n+1}}{\omega(x)}D^{n-1}\omega(x) \\
&= 2x\frac{(-1)^n}{\omega(x)}D^n\omega(x) - 2n\frac{(-1)^{n-1}}{\omega(x)}D^{n-1}\omega(x)
\end{aligned}$$

which implies that

$$\boxed{H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)}, \quad n = 0, 1, 2, \dots \quad (3.19)$$

Combine Eq. (3.13) with Eq. (3.18), and combine Eq. (3.14) with Eq. (3.19), we find that the Hermite polynomials constitute an Appell sequence², i.e., they are a polynomial sequence satisfying the identity [7]

$$He'_n(x) = nHe_{n-1}(x), \quad n = 0, 1, 2, \dots \quad (3.20)$$

$$H'_n(x) = 2nH_{n-1}(x), \quad n = 0, 1, 2, \dots \quad (3.21)$$

Differentiation of Eq. (3.14) gives

$$H'_{n+1}(x) = 2H_n(x) + 2xH'_n(x) - H''_n(x), \quad n = 0, 1, 2, \dots \quad (3.22)$$

Combine with the Appell sequence shown in Eq. (3.20), we have

$$2(n+1)H_n(x) = 2H_n(x) + 2xH'_n(x) - H''_n(x), \quad n = 0, 1, 2, \dots \quad (3.23)$$

Thus

$$H''_n(x) - 2xH'_n(x) + 2nH_n(x) = 0, \quad n = 0, 1, 2, \dots \quad (3.24)$$

which implies that $H_n(x)$ satisfies the second order linear differential equation

$$y''(x) - 2xy'(x) + 2ny(x) = 0, \quad n \in \{0, 1, 2, \dots\} \quad (3.25)$$

²In mathematics, an Appell sequence is any polynomial sequence $\{p_n(x)\}_{n=0,1,2,\dots}$ satisfying the identity $\frac{d}{dx}p_n(x) = np_{n-1}(x)$, and in which $p_0(x)$ is a non-zero constant. Among the most notable Appell sequences besides the trivial example $\{x^n\}$ are the Hermite polynomials, the Bernoulli polynomials, and the Euler polynomials. Every Appell sequence is a Sheffer sequence, but most Sheffer sequences are not Appell sequences.

3.1.1.3 Summary of Properties of the Hermite Polynomials

(1) Orthogonality

He_n and H_n are n th-degree polynomials for $n = 1, 2, 3, \dots$. These polynomials are orthogonal with respect to the weight function (measure) $\omega(x) = e^{-x^2/2}$ for He_n or $\omega(x) = e^{-x^2}$ for H_n . And we have

$$\int_{-\infty}^{\infty} e^{-x^2/2} He_m(x) He_n(x) dx = \sqrt{2\pi} n! \delta_{nm}, \quad m, n \in \{0, 1, 2, \dots\} \quad (3.26a)$$

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx = \sqrt{\pi} 2^n n! \delta_{nm}, \quad m, n \in \{0, 1, 2, \dots\} \quad (3.26b)$$

where δ_{nm} is the Kronecker delta. The probabilist polynomials are thus orthogonal with respect to the standard normal probability density function (standard normal distribution is discussed in Definition 2.1.1).

(2) Recursion Relation

Hermite polynomials satisfy the following recurrence relation

$$He_{n+1}(x) = x He_n(x) - n He_{n-1}(x) \quad (3.27a)$$

$$H_{n+1}(x) = 2x H_n(x) - 2n H_{n-1}(x) \quad (3.27b)$$

For example, from the recursion formulas of the physicists' Hermite polynomials, we have

$$H_{n+1}(x) = (2x - \frac{d}{dx}) H_n(x) \quad (3.28)$$

verify that the formula is valid for $n = 0$, i.e., that

$$H_1(x) = 2x H_0(x) - H_0'(x) \quad (3.29)$$

Since $H_0(x) = 1$ and $H_1(x) = 2x$, this equation is clearly satisfied.

(3) Even/Odd Functions

Notice that the Hermite polynomials in Fig. 3.1 oscillate from even to odd. We can take advantage of that aspect in our calculation of Harmonic Oscillator wave-functions. Hermite Polynomial is an even or odd function depends on its degree n . Based on

$$H_n(-x) = (-1)^n H_n(x) \quad (3.30)$$

$H_n(x)$ is an even function, when n is even; $H_n(x)$ is an odd function, when n is odd.

(4) Integration over Odd/Even Functions

You often consider integrals of the form

$$I = \int_{-a}^a f(x) dx$$

If f is odd or even, then sometimes you can make solving this integral easier. For example, we can rewrite that integral in the following way:

$$\begin{aligned} I &= \int_{-a}^a f(x) dx = \int_{-a}^0 f(x) dx + \int_0^a f(x) dx \\ &= \int_0^a f(-x) dx + \int_0^a f(x) dx \end{aligned}$$

For an even function, we have $f(-x) = f(x)$, whence

$$I = 2 \int_0^a f(x) dx$$

For an odd function, we have $f(-x) = -f(x)$, whence

$$I = 0$$

That's what it means to simplify the integration: the integral of an odd or even function over the interval $[-a, a]$ can be put into a nicer form, and sometimes we can see that it vanishes without even computing an integral.

More generally, if $\lim_{a \rightarrow \infty} \int_{-a}^a |f(x)| dx$ is finite, we have:

$$\int_{-\infty}^{\infty} f(x) dx = \lim_{a \rightarrow \infty} \int_{-a}^a f(x) dx \quad (3.31)$$

Consider an odd function f defined over the entire real line \mathbb{R} . By odd, we mean that $f(-x) = -f(x)$ for all $x \in \mathbb{R}$. We know that integrating an odd function over any symmetric interval of the form $[-a, a]$ gives the value 0. So, if $\lim_{a \rightarrow \infty} \int_{-a}^a |f(x)| dx$ is finite, we get

$$\int_{-\infty}^{\infty} f(x) dx = \lim_{a \rightarrow \infty} \int_{-a}^a f(x) dx = 0 \quad (3.32)$$

For example, for the Hermite polynomials $H_n(x)$, the relevant inner product

$$\langle f, g \rangle = \int_{-\infty}^{\infty} e^{-x^2} f(x) g(x) dx \quad (3.33)$$

While the $H_2(x)H_3(x)$ product is indeed an odd function, while $\exp(-x^2)$ is even. Their product is odd, and thus $\langle f, g \rangle$ certainly ought to be zero.

3.1.2 Construction of Hermite Polynomials

In this section, we will construct the Hermite polynomials in the lattice Boltzmann framework. The probabilists' version He_n with leading coefficient 1 will be used (refer to Definition 3.1.1). From now on, $He_n(x)$ will be denoted by $\mathcal{H}^{(n)}(x)$ in scalar form in 1-dimensional space, and in D -dimensional space, we extend $He_n(x)$ in scalar form to $\mathcal{H}^{(n)}(\xi)$ in tensorial form.

3.1.2.1 Hermite Polynomials in 1-Dimensional Space

In 1-dimensional Cartesian coordinates (x) , the weight function associated with the Hermite polynomials is [8]

$$\omega(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \quad (3.34)$$

The n th-order Hermite polynomial is defined by the Rodrigues formula

$$\mathcal{H}^{(n)}(x) = (-1)^n \frac{1}{\omega(x)} \frac{d^n}{dx^n} \omega(x) \quad (3.35)$$

where $n \geq 0$ is an integer. Again, the first six of these polynomials are

$$\mathcal{H}^{(0)}(x) = 1 \quad (3.36a)$$

$$\mathcal{H}^{(1)}(x) = x \quad (3.36b)$$

$$\mathcal{H}^{(2)}(x) = x^2 - 1 \quad (3.36c)$$

$$\mathcal{H}^{(3)}(x) = x^3 - 3x \quad (3.36d)$$

$$\mathcal{H}^{(4)}(x) = x^4 - 6x^2 + 3 \quad (3.36e)$$

$$\mathcal{H}^{(5)}(x) = x^5 - 10x^3 + 15x \quad (3.36f)$$

Now we derive $\mathcal{H}^{(1)}(x)$ and $\mathcal{H}^{(4)}(x)$ as an example.

$$\begin{aligned} \mathcal{H}^{(1)}(x) &= (-1)^1 \left(\sqrt{2\pi} e^{x^2/2} \right) \frac{d}{dx} \left(\frac{1}{\sqrt{2\pi}} e^{-x^2/2} \right) \\ &= -e^{x^2/2} (-x) e^{-x^2/2} \\ &= x \end{aligned}$$

$$\begin{aligned} \mathcal{H}^{(4)}(x) &= (-1)^4 \left(\sqrt{2\pi} e^{x^2/2} \right) \frac{d^4}{dx^4} \left(\frac{1}{\sqrt{2\pi}} e^{-x^2/2} \right) \\ &= e^{x^2/2} \frac{d^4}{dx^4} \left(e^{-x^2/2} \right) \\ &= e^{x^2/2} \frac{d^3}{dx^3} \left(-x e^{-x^2/2} \right) \\ &= -e^{x^2/2} \frac{d^2}{dx^2} \left(e^{-x^2/2} - x^2 e^{-x^2/2} \right) \\ &= -e^{x^2/2} \frac{d}{dx} \left(-x e^{-x^2/2} - 2x e^{-x^2/2} + x^3 e^{-x^2/2} \right) \\ &= -e^{x^2/2} \frac{d}{dx} \left(-3e^{-x^2/2} + 3x^2 e^{-x^2/2} + 3x^2 e^{-x^2/2} - x^4 e^{-x^2/2} \right) \\ &= x^4 - 6x^2 + 3 \end{aligned}$$

3.1.2.2 Hermite Polynomials in D -Dimensional Space

We can extend the Hermite polynomials definition to D spatial dimensions. The subject of Hermite polynomials in high dimensions has been extensively treated by Grad [1]. In D -dimensional Cartesian coordinates $\boldsymbol{\xi} = (\xi_1, \xi_2, \dots, \xi_D)$, the weight function associated with the Hermite polynomials is

$$\omega(\boldsymbol{\xi}) = \frac{1}{(2\pi)^{D/2}} e^{-\boldsymbol{\xi}^2/2} \quad (3.37)$$

where $\boldsymbol{\xi}^2 = \boldsymbol{\xi} \cdot \boldsymbol{\xi} = \xi_1^2 + \xi_2^2 + \dots + \xi_D^2 = |\boldsymbol{\xi}|^2$. Again, the n th-order Hermite polynomial is defined by the Rodrigues formula

$$\mathcal{H}^{(n)}(\xi) = \frac{(-1)^n}{\omega(\xi)} \nabla^{(n)} \omega(\xi) \quad (3.38)$$

Note that both $\mathcal{H}^{(n)}$ and $\nabla^{(n)}$ are tensors of rank n , i.e. we can represent $\mathcal{H}^{(n)}$ and $\nabla^{(n)}$ by their D^n (from now on, D^n means dimension D with power of n , instead of n th order of derivatives) components: $\mathcal{H}_{\alpha_1 \dots \alpha_n}^{(n)}$ and $\nabla_{\xi_{\alpha_1} \dots \xi_{\alpha_n}}^{(n)}$, respectively, where $\{\alpha_1, \dots, \alpha_n\}$ are n indices running from 1 to D each, i.e. $\alpha_1 \in \{1, \dots, D\}, \dots, \alpha_n \in \{1, \dots, D\}$. Specially, for a 3-dimensional space, $\alpha_1 \in \{x, y, z\}, \dots, \alpha_n \in \{x, y, z\}$. And $\nabla_{\xi_{\alpha_1} \dots \xi_{\alpha_n}}^{(n)}$ is a short notation for n consecutive spatial derivatives:

$$\nabla_{\xi_{\alpha_1} \dots \xi_{\alpha_n}}^{(n)} = \frac{\partial}{\partial \xi_{\alpha_1}} \dots \frac{\partial}{\partial \xi_{\alpha_n}} \quad (3.39)$$

Derivatives are symmetric upon permutation of the indices if we assume that derivatives commute³, e.g. for $D = 3$, $\nabla_{xxy}^{(3)} = \frac{\partial^3}{\partial x \partial x \partial y} = \partial_x^2 \partial_y = \nabla_{xyx}^{(3)} = \frac{\partial^3}{\partial x \partial y \partial x} = \partial_x \partial_y \partial_x = \nabla_{yxx}^{(3)} = \frac{\partial^3}{\partial y \partial x \partial x} = \partial_y \partial_x^2$.

To make this clearer, we explicitly write down the 2-dimensional ($D = 2$) Hermite polynomials up to second order $n = 0, 1, 2$. In the weight function, we have $\xi^2 = \xi \cdot \xi = (\xi_x, \xi_y) \cdot (\xi_x, \xi_y) = \xi_x^2 + \xi_y^2$ (note that here $\{x, y\}$ are just the directions which are the same as $\{1, 2\}$, respectively, since $D = 2$, do not mess them with the position vector \mathbf{x}). Thus (by using array notation, note the use of the array notation should be used sparingly since it can makes the algebra unwieldy and the notation becomes almost unmanageable for tensors of rank higher than two):

For $n = 0$:

$$\begin{aligned} \mathcal{H}^{(0)}(\xi) &= \mathcal{H}^{(0)}(\xi) \\ &= (-1)^0 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla^{(0)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \\ &= 1 \end{aligned}$$

For $n = 1$:

³This is the case for sufficiently smooth functions.

$$\begin{aligned}
\mathcal{H}^{(1)}(\xi) &= \begin{bmatrix} \mathcal{H}_x^{(1)}(\xi) \\ \mathcal{H}_y^{(1)}(\xi) \end{bmatrix} \\
&= \begin{bmatrix} (-1)^1 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_x}^{(1)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \\ (-1)^1 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_y}^{(1)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \end{bmatrix} \\
&= \begin{bmatrix} - \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial}{\partial \xi_x} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \\ - \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial}{\partial \xi_y} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \end{bmatrix} \\
&= \begin{bmatrix} - \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ -\xi_x e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \\ - \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ -\xi_y e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \end{bmatrix} \\
&= \begin{bmatrix} \xi_x \\ \xi_y \end{bmatrix}
\end{aligned}$$

For $n = 2$:

$$\begin{aligned}
\mathcal{H}^{(2)}(\xi) &= \begin{bmatrix} \mathcal{H}_{xx}^{(2)}(\xi) & \mathcal{H}_{xy}^{(2)}(\xi) \\ \mathcal{H}_{yx}^{(2)}(\xi) & \mathcal{H}_{yy}^{(2)}(\xi) \end{bmatrix} \\
&= \begin{bmatrix} (-1)^2 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_x \xi_x}^{(2)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & (-1)^2 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_x \xi_y}^{(2)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \\ (-1)^2 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_y \xi_x}^{(2)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & (-1)^2 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_y \xi_y}^{(2)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \end{bmatrix} \\
&= \begin{bmatrix} \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial^2}{\partial \xi_x \partial \xi_x} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial^2}{\partial \xi_x \partial \xi_y} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \\ \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial^2}{\partial \xi_y \partial \xi_x} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial^2}{\partial \xi_y \partial \xi_y} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \end{bmatrix} \\
&= \begin{bmatrix} \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ (\xi_x^2 - 1) e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ (\xi_x \xi_y) e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \\ \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ (\xi_x \xi_y) e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ (\xi_y^2 - 1) e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \end{bmatrix} \\
&= \begin{bmatrix} \xi_x^2 - 1 & \xi_x \xi_y \\ \xi_x \xi_y & \xi_y^2 - 1 \end{bmatrix}
\end{aligned}$$

For $n = 3$: There are totally 8 third-order Hermite polynomials for $D = 2$, we can denote them as $\mathcal{H}_{\alpha\beta\gamma}^{(3)}$, with $\alpha \in \{x, y\}$, $\beta \in \{x, y\}$ and $\gamma \in \{x, y\}$. Since the components comprise a 3-dimensional matrix (third rank tensor, contains $D^3 = 2^3 = 8$ components), we consider $\mathcal{H}_{x\beta\gamma}^{(3)}$ and $\mathcal{H}_{y\beta\gamma}^{(3)}$ separately.

First, we consider $\mathcal{H}_{x\beta\gamma}^{(3)}$ as follows

$$\begin{aligned}
\mathcal{H}_{x\beta\gamma}^{(3)}(\xi) &= \begin{bmatrix} \mathcal{H}_{xxx}^{(2)}(\xi) & \mathcal{H}_{xxy}^{(2)}(\xi) \\ \mathcal{H}_{xyx}^{(2)}(\xi) & \mathcal{H}_{xyy}^{(2)}(\xi) \end{bmatrix} \\
&= \begin{bmatrix} (-1)^3 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_x \xi_x \xi_x}^{(2)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & (-1)^3 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_x \xi_x \xi_y}^{(2)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \\ (-1)^3 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_x \xi_y \xi_x}^{(2)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & (-1)^3 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_x \xi_y \xi_y}^{(2)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \end{bmatrix} \\
&= \begin{bmatrix} -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial^3}{\partial \xi_x \partial \xi_x \partial \xi_x} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial^3}{\partial \xi_x \partial \xi_x \partial \xi_y} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \\ -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial^3}{\partial \xi_x \partial \xi_y \partial \xi_x} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial^3}{\partial \xi_x \partial \xi_y \partial \xi_y} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \end{bmatrix} \\
&= \begin{bmatrix} -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ (3\xi_x - \xi_x^3) e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \xi_y (1 - \xi_x^2) e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \\ -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \xi_y (1 - \xi_x^2) e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \xi_x (1 - \xi_y^2) e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \end{bmatrix} \\
&= \begin{bmatrix} \xi_x^3 - 3\xi_x & \xi_y(\xi_x^2 - 1) \\ \xi_y(\xi_x^2 - 1) & \xi_x(\xi_y^2 - 1) \end{bmatrix}
\end{aligned}$$

Second, we consider $\mathcal{H}_{y\beta\gamma}^{(3)}$ as follows

$$\begin{aligned}
\mathcal{H}_{y\beta\gamma}^{(3)}(\xi) &= \begin{bmatrix} \mathcal{H}_{yxx}^{(2)}(\xi) & \mathcal{H}_{yxy}^{(2)}(\xi) \\ \mathcal{H}_{yyx}^{(2)}(\xi) & \mathcal{H}_{yyy}^{(2)}(\xi) \end{bmatrix} \\
&= \begin{bmatrix} (-1)^3 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_y \xi_x \xi_x}^{(2)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & (-1)^3 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_y \xi_x \xi_y}^{(2)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \\ (-1)^3 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_y \xi_y \xi_x}^{(2)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & (-1)^3 \left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \nabla_{\xi_y \xi_y \xi_y}^{(2)} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \end{bmatrix} \\
&= \begin{bmatrix} -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial^3}{\partial \xi_y \partial \xi_x \partial \xi_x} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial^3}{\partial \xi_y \partial \xi_x \partial \xi_y} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \\ -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial^3}{\partial \xi_y \partial \xi_y \partial \xi_x} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \frac{\partial^3}{\partial \xi_y \partial \xi_y \partial \xi_y} e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \end{bmatrix} \\
&= \begin{bmatrix} -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \xi_y (1 - \xi_x^2) e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \xi_x (1 - \xi_y^2) e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \\ -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ \xi_x (1 - \xi_y^2) e^{-(\xi_x^2 + \xi_y^2)/2} \right\} & -\left\{ e^{(\xi_x^2 + \xi_y^2)/2} \right\} \left\{ (3\xi_y - \xi_y^3) e^{-(\xi_x^2 + \xi_y^2)/2} \right\} \end{bmatrix} \\
&= \begin{bmatrix} \xi_y(\xi_x^2 - 1) & \xi_x(\xi_y^2 - 1) \\ \xi_x(\xi_y^2 - 1) & \xi_y^3 - 3\xi_y \end{bmatrix}
\end{aligned}$$

Note that if $D = 3$, the second order Hermite polynomials ($n = 2$) form a 3×3 plane matrix (3-dimensional second rank tensor with $D^2 = 3^2 = 9$ components), which will be easy to proof as:

$$\begin{aligned}
\mathcal{H}^{(2)}(\xi) &= \begin{bmatrix} \mathcal{H}_{xx}^{(2)}(\xi) & \mathcal{H}_{xy}^{(2)}(\xi) & \mathcal{H}_{xz}^{(2)}(\xi) \\ \mathcal{H}_{yx}^{(2)}(\xi) & \mathcal{H}_{yy}^{(2)}(\xi) & \mathcal{H}_{yz}^{(2)}(\xi) \\ \mathcal{H}_{zx}^{(2)}(\xi) & \mathcal{H}_{zy}^{(2)}(\xi) & \mathcal{H}_{zz}^{(2)}(\xi) \end{bmatrix} \\
&= \begin{bmatrix} \xi_x^2 - 1 & \xi_x \xi_y & \xi_x \xi_z \\ \xi_x \xi_y & \xi_y^2 - 1 & \xi_y \xi_z \\ \xi_x \xi_z & \xi_y \xi_z & \xi_z^2 - 1 \end{bmatrix}
\end{aligned}$$

And the third order Hermite polynomials ($n = 3$) for $D = 3$ will be a $3 \times 3 \times 3$ cube matrix. We can

say that in a general D -dimensional space, the **second order Hermite polynomials** form a $D \times D$ plane matrix (D -dimensional second rank tensor, which has D^2 components), and the **third order Hermite polynomials** form a $D \times D \times D$ cube matrix (D -dimensional third rank tensor, which has D^3 components). Although higher order Hermite polynomials are hard to imagine geometrically, but we can express them using mathematical notations. The results of $D = 2$ or $D = 3$ can be extended to higher dimensional space. For a general D -dimensional space, the Hermite polynomials (for $n = 1, 2, 3$) can be expressed as follows.

The D -dimensional abscissae vector is $\xi = (\xi_1, \xi_2, \dots, \xi_D)$. Then, the n th-order Hermite polynomials $\mathcal{H}^{(n)}(\xi)$ in a D -dimensional space is an n th rank symmetric tensor and an n th degree polynomial in ξ . The first few polynomials are [1, 9, 10]:

$$\mathcal{H}^{(0)}(\xi) = 1 \quad (3.40a)$$

$$\mathcal{H}_\alpha^{(1)}(\xi) = \xi_\alpha \quad (3.40b)$$

$$\mathcal{H}_{\alpha\beta}^{(2)}(\xi) = \xi_\alpha \xi_\beta - \delta_{\alpha\beta} \quad (3.40c)$$

$$\mathcal{H}_{\alpha\beta\gamma}^{(3)}(\xi) = \xi_\alpha \xi_\beta \xi_\gamma - (\xi_\alpha \delta_{\beta\gamma} + \xi_\beta \delta_{\alpha\gamma} + \xi_\gamma \delta_{\alpha\beta}) \quad (3.40d)$$

where $\delta_{\alpha\beta}$, $\delta_{\beta\gamma}$, in which, $\delta_{\alpha\gamma}$ are the Kronecker delta, with $\alpha \in \{1, 2, \dots, D\}$, $\beta \in \{1, 2, \dots, D\}$ and $\gamma \in \{1, 2, \dots, D\}$. or in tensor notation:

$$\mathcal{H}^{(0)}(\xi) = 1 \quad (3.41a)$$

$$\mathcal{H}^{(1)}(\xi) = \xi \quad (3.41b)$$

$$\mathcal{H}^{(2)}(\xi) = \xi^2 - \delta \quad (3.41c)$$

$$\mathcal{H}^{(3)}(\xi) = \xi^3 - \xi\delta \quad (3.41d)$$

Note that δ is the identity matrix (Kronecker delta), which is always a D -dimensional second rank tensor with $D \times D = D^2$ components.

3.1.3 Orthogonality and Series Expansion

One of the nice features of the Hermite polynomials is their orthogonality. In 1-dimensional, Hermite polynomials are orthogonal with respect to the weight function $\omega(x)$ shown in Eq. (3.34):

$$\int_{-\infty}^{\infty} \omega(x) \mathcal{H}^{(n)}(x) \mathcal{H}^{(m)}(x) dx = n! \delta_{nm} \quad (3.42)$$

where δ_{nm} is the Kronecker delta.

For 1-dimensional space, consider the Gaussian integrals in Section 1.3.2, $\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$, $\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{1}{2a} \sqrt{\frac{\pi}{a}}$, $\int_{-\infty}^{\infty} x^4 e^{-ax^2} dx = \frac{3}{4a^2} \sqrt{\frac{\pi}{a}}$ and $\int_{-\infty}^{\infty} x^6 e^{-ax^2} dx = \frac{15}{8a^3} \sqrt{\frac{\pi}{a}}$, we have the following examples

$$\begin{aligned}
\int_{-\infty}^{\infty} \omega(x) \mathcal{H}^{(0)}(x) \mathcal{H}^{(2)}(x) dx &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \mathcal{H}^{(0)}(x) \mathcal{H}^{(2)}(x) dx \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (1)(x^2 - 1)e^{-x^2/2} dx \\
&= \frac{1}{\sqrt{2\pi}} \left(\int_{-\infty}^{\infty} x^2 e^{-x^2/2} dx - \int_{-\infty}^{\infty} e^{-x^2/2} dx \right) \\
&= \frac{1}{\sqrt{2\pi}} (\sqrt{2\pi} - \sqrt{2\pi}) = 0 \\
\int_{-\infty}^{\infty} \omega(x) \mathcal{H}^{(1)}(x) \mathcal{H}^{(3)}(x) dx &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \mathcal{H}^{(1)}(x) \mathcal{H}^{(3)}(x) dx \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (x)(x^3 - 3x)e^{-x^2/2} dx \\
&= \frac{1}{\sqrt{2\pi}} \left(\int_{-\infty}^{\infty} x^4 e^{-x^2/2} dx - \int_{-\infty}^{\infty} 3x^2 e^{-x^2/2} dx \right) \\
&= \frac{1}{\sqrt{2\pi}} (3\sqrt{2\pi} - 3\sqrt{2\pi}) = 0 \\
\int_{-\infty}^{\infty} \omega(x) \mathcal{H}^{(2)}(x) \mathcal{H}^{(3)}(x) dx &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \mathcal{H}^{(2)}(x) \mathcal{H}^{(3)}(x) dx \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (x^2 - 1)(x^3 - 3x)e^{-x^2/2} dx \\
&= \frac{1}{\sqrt{2\pi}} \left(\int_{-\infty}^{\infty} x^5 e^{-x^2/2} dx - \int_{-\infty}^{\infty} 4x^3 e^{-x^2/2} dx + \int_{-\infty}^{\infty} 3x e^{-x^2/2} dx \right) \\
&= \frac{1}{\sqrt{2\pi}} (0) = 0 \quad (\text{integral of odd functions}) \\
\int_{-\infty}^{\infty} \omega(x) \mathcal{H}^{(3)}(x) \mathcal{H}^{(3)}(x) dx &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \mathcal{H}^{(3)}(x) \mathcal{H}^{(3)}(x) dx \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (x^3 - 3x)(x^3 - 3x)e^{-x^2/2} dx \\
&= \frac{1}{\sqrt{2\pi}} \left(\int_{-\infty}^{\infty} x^6 e^{-x^2/2} dx - \int_{-\infty}^{\infty} 6x^4 e^{-x^2/2} dx + \int_{-\infty}^{\infty} 9x^2 e^{-x^2/2} dx \right) \\
&= \frac{1}{\sqrt{2\pi}} (15\sqrt{2\pi} - 18\sqrt{2\pi} + 9\sqrt{2\pi}) = 6 = 3!
\end{aligned}$$

The orthogonality of the Hermite polynomials can be generalized to D dimensions:

$$\int \omega(\boldsymbol{\xi}) \mathcal{H}_{\boldsymbol{\alpha}}^{(n)}(\boldsymbol{\xi}) \mathcal{H}_{\boldsymbol{\beta}}^{(m)}(\boldsymbol{\xi}) d\boldsymbol{\xi} = \left\{ \prod_{i=1}^D (n_i!) \right\} \delta_{nm} \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}} \quad (3.43)$$

Here, $d\boldsymbol{\xi} = d\xi_1 d\xi_2 \cdots d\xi_D$, and $\delta_{\boldsymbol{\alpha}\boldsymbol{\beta}}$ is a generalized Kronecker delta which is 1 only if $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n)$ is a permutation of $\boldsymbol{\beta} = (\beta_1, \dots, \beta_m)$ and 0 otherwise. There are D^n instances represented by $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n)$ and D^m instances represented by $\boldsymbol{\beta} = (\beta_1, \dots, \beta_m)$, in which both

$\alpha_1 \in \{1, 2, \dots, D\}, \dots, \alpha_n \in \{1, 2, \dots, D\}$ and $\beta_1 \in \{1, 2, \dots, D\}, \dots, \beta_m \in \{1, 2, \dots, D\}$, and they will become the subscripts of the D -dimensional abscissae $\xi = (\xi_1, \xi_2, \dots, \xi_D)$. For example, (x, x, z, y) is a permutation of (y, x, z, x) but not of (x, y, x, y) . And n_i is the number of occurrence of i , in which $i \in \{1, 2, \dots, D\}$. For instance, in a 3-dimensional space with $D = 3$, if $\alpha = (1, 1, 2) = (x, x, y)$ one gets $n_1 = n_x = 2$, $n_2 = n_y = 1$ and $n_3 = n_z = 0$.

For a 3-dimensional space with $D = 3$ in particular, Eq. (3.43) reads

$$\int \omega(\xi) \mathcal{H}_\alpha^{(n)}(\xi) \mathcal{H}_\beta^{(m)}(\xi) d\xi = (n_x!)(n_y!)(n_z!) \delta_{nm} \delta_{\alpha\beta} \quad (3.44)$$

Here, $d\xi = d\xi_x d\xi_y d\xi_z$, and $\delta_{\alpha\beta}$ is a generalized Kronecker delta which is 1 only if $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ is a permutation of $\beta = (\beta_1, \beta_2, \beta_3)$ and 0 otherwise. Similar to D -dimensional space, there are 3^n instances represented by $\alpha = (\alpha_1, \dots, \alpha_n)$ and 3^m instances represented by $\beta = (\beta_1, \dots, \beta_m)$, in which both $\alpha_1 \in \{x, y, z\}, \dots, \alpha_n \in \{x, y, z\}$ and $\beta_1 \in \{x, y, z\}, \dots, \beta_m \in \{x, y, z\}$, and they will become the subscripts of the 3-dimensional abscissae $\xi = (\xi_x, \xi_y, \xi_z)$.

We consider some concrete examples of Eq. (3.44) (note that the z component of the Hermite polynomials was not explicitly appears in the examples, so they are actually 2-dimensional cases with the z direction solely the integral of the weight function). Note that for 3-dimensional space, $\xi^2 = \xi \cdot \xi = \xi_x^2 + \xi_y^2 + \xi_z^2$ in the weight function shown in Eq. (3.37).

The following integrals vanish because the indices α are no permutations of β although the order of both Hermite polynomials is identical ($m = n$), by considering the Gaussian integrals in Section

1.3.2 (in 1-dimensional space), $\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$:

$$\begin{aligned} \int \omega(\xi) \mathcal{H}_x^{(1)}(\xi) \mathcal{H}_y^{(1)}(\xi) d\xi &= \iiint_{-\infty}^{\infty} \frac{1}{(2\pi)^{3/2}} e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} \mathcal{H}_x^{(1)}(\xi) \mathcal{H}_y^{(1)}(\xi) d\xi_x d\xi_y d\xi_z \\ &= \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} \xi_x \xi_y e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} d\xi_x d\xi_y d\xi_z \\ &= \frac{1}{(2\pi)^{3/2}} \left(\int_{-\infty}^{\infty} \xi_x e^{-\xi_x^2/2} d\xi_x \int_{-\infty}^{\infty} \xi_y e^{-\xi_y^2/2} d\xi_y \int_{-\infty}^{\infty} e^{-\xi_z^2/2} d\xi_z \right) \\ &= \frac{1}{(2\pi)^{3/2}} \left((0) \cdot (0) \cdot \sqrt{2\pi} \right) = 0 \quad (\text{integral of odd functions}) \\ \int \omega(\xi) \mathcal{H}_{xy}^{(2)}(\xi) \mathcal{H}_{xx}^{(2)}(\xi) d\xi &= \iiint_{-\infty}^{\infty} \frac{1}{(2\pi)^{3/2}} e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} \mathcal{H}_{xy}^{(2)}(\xi) \mathcal{H}_{xx}^{(2)}(\xi) d\xi_x d\xi_y d\xi_z \\ &= \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} (\xi_x \xi_y) (\xi_x^2 - 1) e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} d\xi_x d\xi_y d\xi_z \\ &= \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} (\xi_x^3 \xi_y) e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} d\xi_x d\xi_y d\xi_z - \\ &\quad \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} (\xi_x \xi_y) e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} d\xi_x d\xi_y d\xi_z \\ &= 0 \quad (\text{leads to integral of odd functions}) \end{aligned}$$

The following integrals vanish because the orders are not identical ($m \neq n$), note the Gaussian integrals in Section 1.3.2 (in 1-dimensional space), $\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$ and $\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{1}{2a} \sqrt{\frac{\pi}{a}}$:

$$\begin{aligned}
\int \omega(\xi) \mathcal{H}_x^{(1)}(\xi) \mathcal{H}_{xy}^{(2)}(\xi) d\xi &= \iiint_{-\infty}^{\infty} \frac{1}{(2\pi)^{3/2}} e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} \mathcal{H}_x^{(1)}(\xi) \mathcal{H}_{xy}^{(2)}(\xi) d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} (\xi_x)(\xi_x \xi_y) e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{(2\pi)^{3/2}} \left(\int_{-\infty}^{\infty} \xi_x^2 e^{-\xi_x^2/2} d\xi_x \int_{-\infty}^{\infty} \xi_y e^{-\xi_y^2/2} d\xi_y \int_{-\infty}^{\infty} e^{-\xi_z^2/2} d\xi_z \right) \\
&= \frac{1}{(2\pi)^{3/2}} \left(\sqrt{2\pi} \cdot (0) \cdot \sqrt{2\pi} \right) = 0
\end{aligned}$$

The following integrals do not vanish since $m = n$ and α is a permutation of β , note that

$$\begin{aligned}
\int_{-\infty}^{\infty} x^4 e^{-ax^2} dx &= \frac{3}{4a^2} \sqrt{\frac{\pi}{a}} \text{ and } \int_{-\infty}^{\infty} x^6 e^{-ax^2} dx = \frac{15}{8a^3} \sqrt{\frac{\pi}{a}}; \\
\int \omega(\xi) \mathcal{H}_x^{(1)}(\xi) \mathcal{H}_x^{(1)}(\xi) d\xi &= \iiint_{-\infty}^{\infty} \frac{1}{(2\pi)^{3/2}} e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} \mathcal{H}_x^{(1)}(\xi) \mathcal{H}_x^{(1)}(\xi) d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} (\xi_x)(\xi_x) e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{(2\pi)^{3/2}} \left(\int_{-\infty}^{\infty} \xi_x^2 e^{-\xi_x^2/2} d\xi_x \int_{-\infty}^{\infty} e^{-\xi_y^2/2} d\xi_y \int_{-\infty}^{\infty} e^{-\xi_z^2/2} d\xi_z \right) \\
&= \frac{1}{(2\pi)^{3/2}} \left(\sqrt{2\pi} \cdot \sqrt{2\pi} \cdot \sqrt{2\pi} \right) \\
&= 1 = 1! = (n_x!)(n_y!)(n_z!) \quad (\text{note that } n_x = 1, n_y = 0, n_z = 0)
\end{aligned}$$

$$\begin{aligned}
\int \omega(\xi) \mathcal{H}_{xxx}^{(3)}(\xi) \mathcal{H}_{xxx}^{(3)}(\xi) d\xi &= \iiint_{-\infty}^{\infty} \frac{1}{(2\pi)^{3/2}} e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} \mathcal{H}_{xxx}^{(3)}(\xi) \mathcal{H}_{xxx}^{(3)}(\xi) d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} (\xi_x^3 - 3\xi_x)(\xi_x^3 - 3\xi_x) e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{(2\pi)^{3/2}} \left(\int_{-\infty}^{\infty} (\xi_x^6 - 6\xi_x^4 + 9\xi_x^2) e^{-\xi_x^2/2} d\xi_x \int_{-\infty}^{\infty} e^{-\xi_y^2/2} d\xi_y \int_{-\infty}^{\infty} e^{-\xi_z^2/2} d\xi_z \right) \\
&= \frac{1}{(2\pi)^{3/2}} \left(\int_{-\infty}^{\infty} \xi_x^6 e^{-\xi_x^2/2} d\xi_x \int_{-\infty}^{\infty} e^{-\xi_y^2/2} d\xi_y \int_{-\infty}^{\infty} e^{-\xi_z^2/2} d\xi_z \right) - \\
&\quad \frac{1}{(2\pi)^{3/2}} \left(\int_{-\infty}^{\infty} 6\xi_x^4 e^{-\xi_x^2/2} d\xi_x \int_{-\infty}^{\infty} e^{-\xi_y^2/2} d\xi_y \int_{-\infty}^{\infty} e^{-\xi_z^2/2} d\xi_z \right) + \\
&\quad \frac{1}{(2\pi)^{3/2}} \left(\int_{-\infty}^{\infty} 9\xi_x^2 e^{-\xi_x^2/2} d\xi_x \int_{-\infty}^{\infty} e^{-\xi_y^2/2} d\xi_y \int_{-\infty}^{\infty} e^{-\xi_z^2/2} d\xi_z \right) \\
&= \frac{1}{(2\pi)^{3/2}} \left(15\sqrt{2\pi} \cdot \sqrt{2\pi} \cdot \sqrt{2\pi} - 18\sqrt{2\pi} \cdot \sqrt{2\pi} \cdot \sqrt{2\pi} + 9\sqrt{2\pi} \cdot \sqrt{2\pi} \cdot \sqrt{2\pi} \right) \\
&= 6 = 3! = (n_x!)(n_y!)(n_z!) \quad (\text{note that } n_x = 3, n_y = 0, n_z = 0)
\end{aligned}$$

$$\begin{aligned}
\int \omega(\boldsymbol{\xi}) \mathcal{H}_{xyx}^{(3)}(\boldsymbol{\xi}) \mathcal{H}_{yxx}^{(3)}(\boldsymbol{\xi}) d\boldsymbol{\xi} &= \iiint_{-\infty}^{\infty} \frac{1}{(2\pi)^{3/2}} e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} \mathcal{H}_{xyx}^{(3)}(\boldsymbol{\xi}) \mathcal{H}_{yxx}^{(3)}(\boldsymbol{\xi}) d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} (\xi_x^2 \xi_y - \xi_y)(\xi_x^2 \xi_y - \xi_y) e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} d\xi_x d\xi_y d\xi_z \\
&= \frac{1}{(2\pi)^{3/2}} \left(\int_{-\infty}^{\infty} (\xi_x^4 - 2\xi_x^2 + 1) e^{-\xi_x^2/2} d\xi_x \int_{-\infty}^{\infty} \xi_y^2 e^{-\xi_y^2/2} d\xi_y \int_{-\infty}^{\infty} e^{-\xi_z^2/2} d\xi_z \right) \\
&= \frac{1}{(2\pi)^{3/2}} \left(\int_{-\infty}^{\infty} \xi_x^4 e^{-\xi_x^2/2} d\xi_x \int_{-\infty}^{\infty} \xi_y^2 e^{-\xi_y^2/2} d\xi_y \int_{-\infty}^{\infty} e^{-\xi_z^2/2} d\xi_z \right) - \\
&\quad \frac{1}{(2\pi)^{3/2}} \left(\int_{-\infty}^{\infty} 2\xi_x^2 e^{-\xi_x^2/2} d\xi_x \int_{-\infty}^{\infty} \xi_y^2 e^{-\xi_y^2/2} d\xi_y \int_{-\infty}^{\infty} e^{-\xi_z^2/2} d\xi_z \right) + \\
&\quad \frac{1}{(2\pi)^{3/2}} \left(\int_{-\infty}^{\infty} e^{-\xi_x^2/2} d\xi_x \int_{-\infty}^{\infty} \xi_y^2 e^{-\xi_y^2/2} d\xi_y \int_{-\infty}^{\infty} e^{-\xi_z^2/2} d\xi_z \right) \\
&= \frac{1}{(2\pi)^{3/2}} \left(3\sqrt{2\pi} \cdot \sqrt{2\pi} \cdot \sqrt{2\pi} - 2\sqrt{2\pi} \cdot \sqrt{2\pi} \cdot \sqrt{2\pi} + \sqrt{2\pi} \cdot \sqrt{2\pi} \cdot \sqrt{2\pi} \right) \\
&= 2 = (2!)(1!) = (n_x!)(n_y!)(n_z!) \quad (\text{note that } n_x = 2, n_y = 1, n_z = 0)
\end{aligned}$$

3.2 Projection onto the Hermite Polynomial Basis

3.2.1 Hermite Series Expansion (Generalized Fourier Series)

3.2.1.1 Background Theory

The 1-dimensional Hermite polynomials form a complete bases in real line \mathbb{R} , The D -dimensional Hermite polynomials form a complete bases in real space \mathbb{R}^D of D dimensions.

The completeness of the $\mathcal{H}^{(n)}(x)$ means that any sufficiently well-behaved function⁴ $f(x) \in \mathbb{R}$ can be represented as a series of Hermite polynomials (a linear combination of the $\mathcal{H}^{(n)}(x)$):

$$\begin{cases} f(x) = \omega(x) \sum_{n=0}^{\infty} \frac{1}{n!} a_n \mathcal{H}^{(n)}(x) \\ a_n = \int f(x) \mathcal{H}^{(n)}(x) dx, \quad n = 0, 1, 2, \dots \infty \end{cases} \quad (3.45)$$

The expansion coefficients a_n are constants. This equation gives us an exact representation of $f(x)$ as an infinite series of Hermite polynomials. We will find we can't use all the infinite number of terms. Rather, we may use only the first five or ten. These finite series will be approximations of $f(x)$.

Again, this can be extended to D dimensions. For any function f such that f/ω is **Square Integrable**⁵, the following **Generalized Fourier Series** exists:

⁴In this discussion, "well behaved" means that $f(x)$ is continuous everywhere except at isolated points where it is permitted to have jump discontinuities.

⁵In mathematics, a square integrable function, also called a L^2 function, is a real-valued or complex-valued measurable function for which the integral of the square of the absolute value is finite. Thus, square-integrability on the real line $(-\infty, +\infty)$ is defined as $\int_{-\infty}^{\infty} |f(x)|^2 dx < \infty$.

$$\begin{cases} f(\xi) = \omega(\xi) \sum_{n=0}^{\infty} \frac{1}{n!} \mathbf{a}^{(n)} : \mathcal{H}^{(n)}(\xi) \\ \mathbf{a}^{(n)} = \int f(\xi) \mathcal{H}^{(n)}(\xi) d\xi, \quad n = 0, 1, 2, \dots, \infty \end{cases} \quad (3.46)$$

where the colon product symbol “:” denotes full tensor contraction. Note that the expansion coefficient $\mathbf{a}^{(n)}$ and Hermite polynomials $\mathcal{H}^{(n)}$ are tensors of rank n . Since $\mathcal{H}^{(n)}$ is a polynomial in ξ , $\mathbf{a}^{(n)}$ are combinations of the velocity moments. Also, we should know that when consider the full dependent variables, $f = f(\mathbf{x}, \xi, t)$, $\mathbf{a}^{(n)} = \mathbf{a}^{(n)}(\mathbf{x}, t)$ and $\mathcal{H}^{(n)} = \mathcal{H}^{(n)}(\xi)$. Thus, in space ξ which is D -dimensional, \mathbf{a}_n are constants.

Theorem 3.2.1 – Generalized Fourier series. A generalized Fourier series is a series expansion of a function based on the special properties of a complete orthogonal system of functions. There are many types of function spaces, such as the Classical Orthogonal Polynomials [11]. Hermite polynomials form a typical infinite dimensional orthogonal function space.

Here we first generalize the dot product. Recall that there are two forms for the dot product in three dimensions (For more general vector spaces the term inner product is used to generalize the notions of dot and scalar products). First, one has that $\mathbf{u} \cdot \mathbf{v} = uv \cos \theta$, where u and v denote the length of the vectors. The other form is the component form: $\mathbf{u} \cdot \mathbf{v} = u_1 v_1 + u_2 v_2 + u_3 v_3 = \sum_{k=1}^3 u_k v_k$.

Of course, this form is easier to generalize. So, we define the scalar product, or inner product, between two n -dimensional vectors as

$$\langle \mathbf{u}, \mathbf{v} \rangle = \sum_{k=1}^n u_k v_k \quad (3.47)$$

Actually, there are a number of notations that are used in other texts. One can write the scalar product as (\mathbf{u}, \mathbf{v}) or even in the Dirac bra-ket notation $\langle \mathbf{u} | \mathbf{v} \rangle$.

We note that the (real) scalar product satisfies some simple properties. For vectors \mathbf{u}, \mathbf{v} and real scalar α we have

$$\langle \mathbf{u}, \mathbf{u} \rangle \geq 0, \text{ and } \langle \mathbf{u}, \mathbf{u} \rangle = 0 \text{ if and only if } \mathbf{u} = 0 \quad (3.48a)$$

$$\langle \mathbf{u}, \mathbf{v} \rangle = \langle \mathbf{v}, \mathbf{u} \rangle \quad (3.48b)$$

$$\langle \alpha \mathbf{u}, \mathbf{v} \rangle = \alpha \langle \mathbf{u}, \mathbf{v} \rangle \quad (3.48c)$$

A real vector space equipped with the above inner product leads to what is called a real **inner product space**. For the time being, we will only deal with real valued functions and, thus we will need an inner product appropriate for such spaces. One such definition is the following. Let $f(x)$ and $g(x)$ be functions defined on $[a, b]$, and introduce the weight function $\omega(x) > 0$. Then, we define the *inner product*, if the integral exists, as

$$\langle f, g \rangle = \int_a^b \omega(x) f(x) g(x) dx \quad (3.49)$$

This is actually identical to the inner product in Definition 3.1.2.

Spaces in which $\langle f, f \rangle < \infty$ under this inner product are called the space of square integrable

functions on (a, b) under weight ω and are denoted as $L_\omega^2(a, b)$. (Note that with the square integrable criterion added, the inner product space criteria defined in Eq. (3.48) can be met.) Sometimes for simplicity, the weight function is assumed $\omega(x) = 1$. This is possible to do using a change of variables.

In mathematical analysis, many generalizations of Fourier series have proved to be useful. They are all special cases of decompositions over an orthonormal basis of an inner product space. Here we consider that of square-integrable functions defined on an interval of the real line, which is important, among others, for interpolation theory.

Now that we have function spaces equipped with an inner product, we seek a basis for the space. For an n -dimensional space we need n basis vectors. For an infinite dimensional space, how many will we need? How do we know when we have enough? We will provide some answers to these questions later.

Let $f(x)$ be represented by an expansion over a basis of **orthogonal functions**, $\Phi = \{\phi_n(x)\}_{n=0}^\infty$, in \mathbb{R} . The **generalized Fourier series** of a square-integrable function f in \mathbb{R} , with respect to Φ , is then [12, 13, 14]

$$f(x) = \sum_{n=0}^{\infty} a_n \phi_n(x) \quad (3.50)$$

Then, the expansion coefficients are formally determined as

$$a_n = \frac{\langle \phi_n, f \rangle}{\langle \phi_n, \phi_n \rangle} = \frac{\langle \phi_n, f \rangle}{\|\phi_n\|^2}, \quad n = 0, 1, 2, \dots, \infty \quad (3.51)$$

This will be referred to as the generalized Fourier series expansion and a_n are called the Fourier coefficients. Technically, equality in the generalized Fourier series only holds when the infinite series converges to the given function on the interval of interest.

Proof: Given a complete orthogonal system of univariate basis functions $\{\phi_n(x)\}_{n=0}^\infty$ over the interval \mathbb{R} , the functions $\phi_n(x)$ satisfy an orthogonality relationship of the form (refer to Definition 3.1.2):

$$\int_{-\infty}^{\infty} \omega(x) \phi_m(x) \phi_n(x) dx = h_n \delta_{nm} \quad (3.52)$$

where h_n are given constants and δ_{nm} is the Kronecker delta.

Consider an arbitrary function being written as a series $f(x) = \sum_{n=0}^{\infty} a_n \phi_n(x)$. Now we are finding the components of f in this basis, i.e. a_n .

We take the inner product of f with each ϕ_j and use the properties of the inner product and orthogonality to obtain

$$\begin{aligned}
\langle \phi_j(x), f(x) \rangle &= \langle \phi_j(x), \sum_{n=0}^{\infty} a_n \phi_n(x) \rangle \\
&= \int_{-\infty}^{\infty} \left\{ \omega(x) \phi_j(x) \sum_{n=0}^{\infty} a_n \phi_n(x) \right\} dx \\
&= \sum_{n=0}^{\infty} \left\{ a_n \int_{-\infty}^{\infty} \omega(x) \phi_j(x) \phi_n(x) dx \right\} \\
&= \sum_{n=0}^{\infty} a_n \langle \phi_j(x), \phi_n(x) \rangle \\
&= \sum_{n=0}^{\infty} a_n h_j \delta_{jn} \\
&= a_j h_j = a_j \langle \phi_j(x), \phi_j(x) \rangle
\end{aligned}$$

Thus all the expansion coefficient can be expressed as $a_n = \frac{\langle \phi_n, f \rangle}{\langle \phi_n, \phi_n \rangle}$, with $n = 0, 1, 2, \dots, \infty$.

Now we can prove the generalized Fourier series for the distribution function based on the Hermite polynomials, as introduced in Eq. (3.45).

We have discussed that the Hermite polynomials $\mathcal{H}^{(n)}(x)$ are orthogonal polynomials on the interval $(-\infty, \infty)$, as defined in Eq. (3.35). Consider a square integrable function $g(x)$, which can be expanded by the generalized Fourier series $g(x) = \sum_{n=0}^{\infty} a_n \mathcal{H}^{(n)}(x)$. We take the inner product of g with each $\mathcal{H}^{(j)}(x)$ and use the properties of the inner product and orthogonality shown in Eq. (3.42), to obtain

$$\begin{aligned}
\langle \mathcal{H}^{(j)}(x), g(x) \rangle &= \langle \mathcal{H}^{(j)}(x), \sum_{n=0}^{\infty} a_n \mathcal{H}^{(n)}(x) \rangle \\
&= \int_{-\infty}^{\infty} \left\{ \omega(x) \mathcal{H}^{(j)}(x) \sum_{n=0}^{\infty} a_n \mathcal{H}^{(n)}(x) \right\} dx \\
&= \sum_{n=0}^{\infty} \left\{ a_n \int_{-\infty}^{\infty} \omega(x) \mathcal{H}^{(j)}(x) \mathcal{H}^{(n)}(x) dx \right\} \\
&= \sum_{n=0}^{\infty} a_n \langle \mathcal{H}^{(j)}(x), \mathcal{H}^{(n)}(x) \rangle \\
&= \sum_{n=0}^{\infty} a_n j! \delta_{jn} \\
&= a_j j! = a_j \langle \mathcal{H}^{(j)}(x), \mathcal{H}^{(j)}(x) \rangle
\end{aligned}$$

So we obtain

$$a_j = \frac{\langle \mathcal{H}^{(j)}(x), g(x) \rangle}{\langle \mathcal{H}^{(j)}(x), \mathcal{H}^{(j)}(x) \rangle} = \frac{\langle \mathcal{H}^{(j)}(x), g(x) \rangle}{j!} = \frac{1}{j!} \int \omega(x) g(x) \mathcal{H}^{(j)}(x) dx \quad (3.53)$$

Now we define the distribution function $f(x) = \omega(x) \sum_{n=0}^{\infty} \frac{1}{n!} a_n \mathcal{H}^{(n)}(x)$, which is a modified generalized Fourier series of $g(x)$ (not that $f(x) \neq \frac{\omega(x)g(x)}{n!}$ since $n!$ in $f(x)$ varies corresponding each summation term), thus we can update the expansion coefficients or the Fourier coefficients as

$$a_j = \frac{1}{j!} \int \omega(x) g(x) \mathcal{H}^{(j)}(x) dx = \int \frac{\omega(x)}{j!} \left\{ \sum_{n=0}^{\infty} a_n \mathcal{H}^{(n)}(x) \right\} \mathcal{H}^{(j)}(x) dx$$

Here, if we move $j!$ into the summation:

$$\sum_{n=0}^{\infty} \frac{1}{j!} a_n \mathcal{H}^{(n)}(x) \neq \sum_{m=0}^{\infty} \frac{1}{n!} a_n \mathcal{H}^{(n)}(x)$$

But we can do it in the expansion coefficient equation since only $n = j$ survive due to the orthogonality property of Hermite polynomials. Thus,

$$a_j = \int \omega(x) \left\{ \sum_{n=0}^{\infty} \frac{1}{n!} a_n \mathcal{H}^{(n)}(x) \right\} \mathcal{H}^{(j)}(x) dx$$

Or we have

$$a_n = \int \omega(x) \left\{ \sum_{m=0}^{\infty} \frac{1}{m!} a_m \mathcal{H}^{(m)}(x) \right\} \mathcal{H}^{(n)}(x) dx = \int f(x) \mathcal{H}^{(n)}(x) dx \quad (3.54)$$

Thus, the generalized Fourier series with 1-dimensional Hermite polynomials as shown in (3.45) can be proved. We will continue to prove the D -dimensional generalized Fourier series here, but the expansion coefficient will be denoted as $\mathbf{a}^{(n)}$ which is a rank n tensor.

The polynomial expansion in Eq. (3.46) can be seen as the decomposition of f onto an orthogonal polynomial basis, since Hermite tensors are orthogonal with respect to the following scalar product (inner product) [15]:

$$\langle g, h \rangle \equiv \langle g|h \rangle = \int \omega(\xi) g(\xi) h(\xi) d\xi \quad (3.55)$$

Thus $\mathbf{a}^{(n)}$ can simply be obtained as a projection of f onto this orthogonal basis $\mathbf{a}^{(n)} = \langle \mathcal{H}^{(n)} | f / \omega \rangle$.

3.2.1.2 Hermite Series Expansion of the General Distribution Function

Evidently from Eq. (3.46), all the expansion coefficients are linear combinations of the velocity moments of f . Specifically, on substituting the explicit expressions of the Hermite polynomials in Eqs. (3.41) into Eq. (3.46), the first few expansion coefficients are directly identified with the familiar hydrodynamic variables, refer to conservation of moments for the general distribution functions discussed in Section 2.1.2 and the equilibrium distribution function discussed in Section

2.1.3:

$$\mathbf{a}^{(0)} = \int f(\boldsymbol{\xi}) \mathcal{H}^{(0)}(\boldsymbol{\xi}) d\boldsymbol{\xi} = \int f(\boldsymbol{\xi}) d\boldsymbol{\xi} = \rho \quad (3.56a)$$

$$\mathbf{a}^{(1)} = \int f(\boldsymbol{\xi}) \mathcal{H}^{(1)}(\boldsymbol{\xi}) d\boldsymbol{\xi} = \int \boldsymbol{\xi} f(\boldsymbol{\xi}) d\boldsymbol{\xi} = \rho \mathbf{u} \quad (3.56b)$$

$$\mathbf{a}^{(2)} = \int f(\boldsymbol{\xi}) \mathcal{H}^{(2)}(\boldsymbol{\xi}) d\boldsymbol{\xi} = \int (\boldsymbol{\xi}^2 - \delta) f(\boldsymbol{\xi}) d\boldsymbol{\xi} = \mathbf{P} + \rho(\mathbf{u}^2 - \delta) \quad (3.56c)$$

$$\mathbf{a}^{(3)} = \int f(\boldsymbol{\xi}) \mathcal{H}^{(3)}(\boldsymbol{\xi}) d\boldsymbol{\xi} = \int (\boldsymbol{\xi}^3 - \boldsymbol{\xi} \delta) f(\boldsymbol{\xi}) d\boldsymbol{\xi} = \mathbf{Q} + \mathbf{u} \mathbf{a}^{(2)} - (D-1) \rho \mathbf{u}^3 \quad (3.56d)$$

δ is the identity matrix (D -dimensional second rank tensor with $D \times D = D^2$ components). As introduced in Eqs (2.14):

$$\mathbf{P} = \int f \mathbf{c}^2 d\boldsymbol{\xi}, \quad \mathbf{Q} = \int f \mathbf{c}^3 d\boldsymbol{\xi} \quad (3.57)$$

in which the intrinsic velocity is defined as $\mathbf{c}(\mathbf{x}, \boldsymbol{\xi}, t) = \boldsymbol{\xi} - \mathbf{u}(\mathbf{x}, t)$ as shown in Eq. (2.12), which means that in the α direction, we have $\xi_\alpha = c_\alpha + u_\alpha$.

Proof: Tensors $\mathbf{a}^{(0)}$ and $\mathbf{a}^{(1)}$ are obvious from the conclusions in Section 2.1.2. Now we proof $\mathbf{a}^{(2)}$ and $\mathbf{a}^{(3)}$ for a D -dimensional space.

From previous discussions we have:

$$\begin{aligned} \mathcal{H}^{(2)}(\boldsymbol{\xi}) &= \boldsymbol{\xi}^2 - \delta = \mathcal{H}_{\alpha\beta}^{(2)}(\boldsymbol{\xi}) = \xi_\alpha \xi_\beta - \delta_{\alpha\beta} = \begin{bmatrix} \mathcal{H}_{xx}^{(2)}(\boldsymbol{\xi}) & \mathcal{H}_{xy}^{(2)}(\boldsymbol{\xi}) \\ \mathcal{H}_{yx}^{(2)}(\boldsymbol{\xi}) & \mathcal{H}_{yy}^{(2)}(\boldsymbol{\xi}) \end{bmatrix} = \begin{bmatrix} \xi_x^2 - 1 & \xi_x \xi_y \\ \xi_x \xi_y & \xi_y^2 - 1 \end{bmatrix} \\ &= \begin{bmatrix} (c_x + u_x)^2 - 1 & (c_x + u_x)(c_y + u_y) \\ (c_x + u_x)(c_y + u_y) & (c_y + u_y)^2 - 1 \end{bmatrix} \\ &= \begin{bmatrix} (c_x c_x) + (2c_x u_x) + (u_x u_x) - 1 & (c_x c_y) + (c_x u_y + c_y u_x) + (u_x u_y) \\ (c_x c_y) + (c_x u_y + c_y u_x) + (u_x u_y) & (c_y c_y) + (2c_y u_y) + (u_y u_y) - 1 \end{bmatrix} \\ &= c_\alpha c_\beta + (c_\alpha u_\beta + c_\beta u_\alpha) + u_\alpha u_\beta - \delta_{\alpha\beta} \quad (\text{for general } D\text{-dimensional space}) \\ &= \mathbf{c}^2 + \left\{ \mathbf{c} \mathbf{u} + (\mathbf{c} \mathbf{u})^T \right\} + \mathbf{u}^2 - \delta \end{aligned}$$

Note that the tensor product of two vectors, denoted by $\mathbf{a} \mathbf{b}$ (sometimes denoted $\mathbf{a} \otimes \mathbf{b}$), produces a second rank tensor.

Actually we can directly obtain this result, as

$$\begin{aligned} \mathcal{H}_{\alpha\beta}^{(2)}(\boldsymbol{\xi}) &= \xi_\alpha \xi_\beta - \delta_{\alpha\beta} \\ &= (c_\alpha + u_\alpha)(c_\beta + u_\beta) - \delta_{\alpha\beta} \\ &= c_\alpha c_\beta + (c_\alpha u_\beta + c_\beta u_\alpha) + u_\alpha u_\beta - \delta_{\alpha\beta} \end{aligned}$$

Since $\int \mathbf{c} f d\boldsymbol{\xi} = 0$, as proved in Section 2.1.2, thus

$$\int \left\{ \mathbf{c} \mathbf{u} + (\mathbf{c} \mathbf{u})^T \right\} f(\boldsymbol{\xi}) d\boldsymbol{\xi} = 0$$

as $\mathbf{u}(\mathbf{x}, t)$ is not a function of $\boldsymbol{\xi}$ and can be moved outside of the integrand. Thus we can prove that:

$$\mathbf{a}^{(2)} = \int (\boldsymbol{\xi}^2 - \boldsymbol{\delta}) f(\boldsymbol{\xi}) d\boldsymbol{\xi} = \int (\mathbf{c}^2 + \mathbf{u}^2 - \boldsymbol{\delta}) f(\boldsymbol{\xi}) d\boldsymbol{\xi} = \mathbf{P} + \rho(\mathbf{u}^2 - \boldsymbol{\delta})$$

Also,

$$\begin{aligned} \mathcal{H}_{\alpha\beta\gamma}^{(3)}(\boldsymbol{\xi}) &= \xi_\alpha \xi_\beta \xi_\gamma - (\xi_\alpha \delta_{\beta\gamma} + \xi_\beta \delta_{\alpha\gamma} + \xi_\gamma \delta_{\alpha\beta}) \\ &= (c_\alpha + u_\alpha)(c_\beta + u_\beta)(c_\gamma + u_\gamma) - \{(c_\alpha + u_\alpha)\delta_{\beta\gamma} + (c_\beta + u_\beta)\delta_{\alpha\gamma} + (c_\gamma + u_\gamma)\delta_{\alpha\beta}\} \\ &= c_\alpha c_\beta c_\gamma + (c_\alpha c_\beta u_\gamma + c_\alpha c_\gamma u_\beta + c_\beta c_\gamma u_\alpha) + (c_\alpha u_\beta u_\gamma + c_\beta u_\alpha u_\gamma + c_\gamma u_\alpha u_\beta) + u_\alpha u_\beta u_\gamma \\ &\quad - (c_\alpha \delta_{\beta\gamma} + c_\beta \delta_{\alpha\gamma} + c_\gamma \delta_{\alpha\beta}) - (u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta}) \\ &= \mathbf{c}^3 + 3\mathbf{c}^2 \mathbf{u} + 3\mathbf{c} \mathbf{u}^2 + \mathbf{u}^3 - \mathbf{c} \boldsymbol{\delta} - \mathbf{u} \boldsymbol{\delta} \end{aligned}$$

Tensors of higher rank than two can be formed by the product of more than two vectors, e.g. a third rank tensor \mathbf{abc} , a fourth rank tensor \mathbf{abcd} , in which $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$ are vectors (a vector is itself a first rank tensor and a scalar is a tensor of rank zero).

CANNOT proof $\mathbf{a}^{(3)}$ currently.

Evidently, the thermodynamic variables can be expressed in terms of the low-order Hermite expansion coefficients:

$$\rho = \mathbf{a}^{(0)} \quad (3.58a)$$

$$\rho \mathbf{u} = \mathbf{a}^{(1)} \quad (3.58b)$$

$$\mathbf{P} = \mathbf{a}^{(2)} - \rho(\mathbf{u}^2 - \boldsymbol{\delta}) \quad (3.58c)$$

$$\mathbf{Q} = \mathbf{a}^{(3)} - \mathbf{u} \mathbf{a}^{(2)} + (D - 1)\rho \mathbf{u}^3 \quad (3.58d)$$

As discussed in Section 2.1.2, $P_{ii} = \text{tr}(P_{ij}) = \sum_{i=1}^D P_{ii} = Dp$. From Section 2.1.5, the non-dimensional parameters $p = \rho\theta$ and the internal energy $e = \frac{D}{2}\theta$ (refer to Section 2.1.5.2), we have $\rho e = \frac{1}{2}Dp$, so we have

$$\rho e = \frac{1}{2}Dp = \frac{1}{2}P_{ii} = \frac{1}{2}\text{tr}(P_{ij}) = \frac{1}{2}\{a_{ii}^{(2)} - \rho(u^2 - D)\} \quad (3.59)$$

Note that the trace of the $D \times D$ identity matrix $\boldsymbol{\delta}$ is the dimension of the space, namely D .

Therefore, the five fundamental thermodynamic variables, ρ , \mathbf{u} and $\theta = 2e/D$, and the momentum flux tensor \mathbf{P} (or its traceless part the stress tensor $\boldsymbol{\sigma}$, which **needs more investigation here**) are completely determined by the first three Hermite expansion coefficients alone, whereas the third moment, i.e. the heat flux \mathbf{q} , is completely determined by the fourth coefficient (**need proof here**).

3.2.1.3 Hermite Series Expansion of the Equilibrium Distribution Function

Let us now apply the Hermite series expansion in Eq. (3.46) to the equilibrium distribution function shown in Eq. (2.41) in $\boldsymbol{\xi}$ -space. The computation of these coefficients $\mathbf{a}^{(n),\text{eq}} = \langle \mathcal{H}^{(n)} | f^{\text{eq}} / \omega \rangle$ is straightforward since the expression of f^{eq} is known.

The equilibrium distribution function $f^{\text{eq}}(\boldsymbol{\xi})$ shown in Eq. (2.41) has the similar form as the weight function $\omega(\boldsymbol{\xi})$ of the Hermite polynomials shown in Eq. (3.37).

$$f^{\text{eq}}(\mathbf{x}, \boldsymbol{\xi}, t) = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left(-\frac{|\boldsymbol{\xi} - \mathbf{u}|^2}{2\theta}\right)$$

$$\omega(\boldsymbol{\xi}) = \frac{1}{(2\pi)^{D/2}} e^{-|\boldsymbol{\xi}|^2/2}$$

with $|\boldsymbol{\xi}|^2 = \boldsymbol{\xi} \cdot \boldsymbol{\xi}$. Since $\omega(\boldsymbol{\xi}) = \frac{1}{(2\pi)^{D/2}} e^{-|\boldsymbol{\xi}|^2/2}$, thus $\omega\left(\frac{\boldsymbol{\xi} - \mathbf{u}}{\theta^{1/2}}\right) = \frac{1}{(2\pi)^{D/2}} e^{-|\boldsymbol{\xi} - \mathbf{u}|^2/2\theta}$, so we have $f^{\text{eq}} = \frac{\rho}{\theta^{D/2}} \omega\left(\frac{\boldsymbol{\xi} - \mathbf{u}}{\theta^{1/2}}\right)$.

The Hermite series expansion coefficient of the Maxwellian:

$$\begin{aligned} \mathbf{a}^{(n),\text{eq}} &= \int f^{\text{eq}}(\boldsymbol{\xi}) \mathcal{H}^{(n)}(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad n = 0, 1, 2, \dots, \infty \\ &= \frac{\rho}{\theta^{D/2}} \int \omega\left(\frac{\boldsymbol{\xi} - \mathbf{u}}{\theta^{1/2}}\right) \mathcal{H}^{(n)}(\boldsymbol{\xi}) d\boldsymbol{\xi} \end{aligned}$$

Apply a change of the variable $(\boldsymbol{\xi} - \mathbf{u})/\sqrt{\theta} = \boldsymbol{\eta} \implies \boldsymbol{\xi} = \sqrt{\theta}\boldsymbol{\eta} + \mathbf{u}$. For a D -dimensional space $\boldsymbol{\xi}$, the D -fold integral indicates $d\boldsymbol{\xi} = d^D\xi = d\xi_1 d\xi_2 \dots d\xi_D$, thus we have $d\boldsymbol{\xi} = \theta^{D/2} d\boldsymbol{\eta}$, then Hermite polynomials coefficients are computed as follows

$$\mathbf{a}^{(n),\text{eq}} = \rho \int \omega(\boldsymbol{\eta}) \mathcal{H}^{(n)}(\sqrt{\theta}\boldsymbol{\eta} + \mathbf{u}) d\boldsymbol{\eta} \quad (3.60)$$

The special attention should be given to the difference between $f^{\text{eq}}(\boldsymbol{\xi})$ and $\omega(\boldsymbol{\xi})$, although they have similar form, since $\omega(\boldsymbol{\xi})$ will be an even function (in each direction) but $f^{\text{eq}}(\boldsymbol{\xi})$ not.

The Hermite series of the equilibrium distribution function will be

$$f^{\text{eq}}(\boldsymbol{\xi}) = \omega(\boldsymbol{\xi}) \sum_{n=0}^{\infty} \frac{1}{n!} \mathbf{a}^{(n),\text{eq}} : \mathcal{H}^{(n)}(\boldsymbol{\xi}) \quad (3.61)$$

The leading Hermite series expansion coefficients (up to the third order) of the Maxwellian are obtained for convenience) by substituting the explicit expressions of the Hermite polynomials in Eqs. (3.41) into Eq. (3.60)

$$\mathbf{a}^{(0),\text{eq}} = \rho \int \omega(\boldsymbol{\eta}) d\boldsymbol{\eta} = \rho \quad (3.62a)$$

$$\mathbf{a}^{(1),\text{eq}} = \rho \int (\sqrt{\theta}\boldsymbol{\eta} + \mathbf{u}) \omega(\boldsymbol{\eta}) d\boldsymbol{\eta} = \rho \mathbf{u} \quad (3.62b)$$

$$\mathbf{a}^{(2),\text{eq}} = \rho \int \left\{ (\sqrt{\theta}\boldsymbol{\eta} + \mathbf{u})^2 - \delta \right\} \omega(\boldsymbol{\eta}) d\boldsymbol{\eta} = \rho \mathbf{u}^2 + \rho(\theta - 1)\delta \quad (3.62c)$$

$$\mathbf{a}^{(3),\text{eq}} = \rho \int \left\{ (\sqrt{\theta}\boldsymbol{\eta} + \mathbf{u})^3 - (\sqrt{\theta}\boldsymbol{\eta} + \mathbf{u})\delta \right\} \omega(\boldsymbol{\eta}) d\boldsymbol{\eta} = \rho \mathbf{u}^3 + \rho(\theta - 1)\mathbf{u}\delta \quad (3.62d)$$

Proof: The proof process will refer to the results in Section 2.1.3.

For $\mathbf{a}^{(0),\text{eq}}$, refer to Gaussian integrals in Section 1.3.2, $\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$, thus

$$\begin{aligned}\mathbf{a}^{(0),\text{eq}} &= \rho \int \omega(\boldsymbol{\eta}) d\boldsymbol{\eta} \\ &= \rho \int \left\{ \frac{1}{(2\pi)^{D/2}} e^{-|\boldsymbol{\eta}|^2/2} \right\} d^D \boldsymbol{\eta} \\ &= \frac{\rho}{(2\pi)^{D/2}} (2\pi)^{D/2} \\ &= \rho\end{aligned}$$

For $\mathbf{a}^{(1),\text{eq}}$, we noticed that the integrand of $\int \boldsymbol{\eta} \omega(\boldsymbol{\eta}) d\boldsymbol{\eta}$ are odd functions (in different directions), which vanishes in the integral. Thus, $\mathbf{a}^{(1),\text{eq}} = \rho \mathbf{u}$ is obvious.

For $\mathbf{a}^{(2),\text{eq}}$, since $\mathcal{H}_{\alpha\beta}^{(2)}(\boldsymbol{\xi}) = \xi_\alpha \xi_\beta - \delta_{\alpha\beta}$, thus

$$\begin{aligned}\mathcal{H}^{(2)}(\sqrt{\theta}\boldsymbol{\eta} + \mathbf{u}) &= (\sqrt{\theta}\boldsymbol{\eta} + \mathbf{u})^2 - \boldsymbol{\delta} \\ &= (\sqrt{\theta}\eta_\alpha + u_\alpha)(\sqrt{\theta}\eta_\beta + u_\beta) - \delta_{\alpha\beta} \\ &= \theta\eta_\alpha\eta_\beta + \sqrt{\theta}\eta_\alpha u_\beta + \sqrt{\theta}\eta_\beta u_\alpha + u_\alpha u_\beta - \delta_{\alpha\beta} \\ &= \theta\boldsymbol{\eta}^2 + \sqrt{\theta}\{\boldsymbol{\eta}\mathbf{u} + (\boldsymbol{\eta}\mathbf{u})^T\} + \mathbf{u}^2 - \boldsymbol{\delta}\end{aligned}$$

Also, consider that $\omega(\boldsymbol{\xi})$ will be an even function in each direction, so integrals with $\sqrt{\theta}\eta_\alpha u_\beta$ and $\sqrt{\theta}\eta_\beta u_\alpha$ as integrand vanish. We will use the Gaussian integral $\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{1}{2a} \sqrt{\frac{\pi}{a}}$ discussed in Section 1.3.2. Thus

$$\begin{aligned}\mathbf{a}^{(2),\text{eq}} &= \rho \int \left\{ (\sqrt{\theta}\boldsymbol{\eta} + \mathbf{u})^2 - \boldsymbol{\delta} \right\} \omega(\boldsymbol{\eta}) d\boldsymbol{\eta} \\ &= \rho \int \left\{ \theta\boldsymbol{\eta}^2 + \mathbf{u}^2 - \boldsymbol{\delta} \right\} \omega(\boldsymbol{\eta}) d\boldsymbol{\eta} \\ &= \rho\theta \int \boldsymbol{\eta}^2 \left\{ \frac{1}{(2\pi)^{D/2}} e^{-|\boldsymbol{\eta}|^2/2} \right\} d^D \boldsymbol{\eta} + \rho(\mathbf{u}^2 - \boldsymbol{\delta})\end{aligned}$$

Here, we use 2-dimensional space as an example,

$$\boldsymbol{\eta}^2 = \eta_\alpha \eta_\beta = \begin{bmatrix} \eta_x \eta_x & \eta_x \eta_y \\ \eta_x \eta_y & \eta_y \eta_y \end{bmatrix}$$

Thus

$$\begin{aligned}\iint \eta_x^2 e^{-(\eta_x^2 + \eta_y^2)/2} d\eta_x d\eta_y &= \int \eta_x^2 e^{-\eta_x^2/2} d\eta_x \int e^{-\eta_y^2/2} d\eta_y \\ &= \sqrt{2\pi} \sqrt{2\pi} = (2\pi)^{D/2}\end{aligned}$$

And

$$\begin{aligned} \iint \eta_x \eta_y e^{-(\eta_x^2 + \eta_y^2)/2} d\eta_x d\eta_y &= \int \eta_x e^{-\eta_x^2/2} d\eta_x \int \eta_y e^{-\eta_y^2/2} d\eta_y \\ &= 0 \quad (\text{integral of odd function}) \end{aligned}$$

Thus

$$\begin{aligned} \int \eta^2 \left\{ \frac{1}{(2\pi)^{D/2}} e^{-|\eta|^2/2} \right\} d\eta &= \delta \quad (\text{identity matrix}) \\ \mathbf{a}^{(2),\text{eq}} &= \rho\theta\delta + \rho(\mathbf{u}^2 - \delta) = \rho\mathbf{u}^2 + \rho(\theta - 1)\delta \end{aligned} \quad (3.63)$$

For $\mathbf{a}^{(3),\text{eq}}$, since $\mathcal{H}_{\alpha\beta\gamma}^{(3)}(\boldsymbol{\xi}) = \xi_\alpha \xi_\beta \xi_\gamma - (\xi_\alpha \delta_{\beta\gamma} + \xi_\beta \delta_{\alpha\gamma} + \xi_\gamma \delta_{\alpha\beta})$, thus

$$\begin{aligned} \mathcal{H}^{(3)}(\sqrt{\theta}\boldsymbol{\eta} + \mathbf{u}) &= (\sqrt{\theta}\boldsymbol{\eta} + \mathbf{u})^3 - (\sqrt{\theta}\boldsymbol{\eta} + \mathbf{u})\delta \\ &= (\sqrt{\theta}\eta_\alpha + u_\alpha)(\sqrt{\theta}\eta_\beta + u_\beta)(\sqrt{\theta}\eta_\gamma + u_\gamma) \\ &\quad - \left\{ (\sqrt{\theta}\eta_\alpha + u_\alpha)\delta_{\beta\gamma} + (\sqrt{\theta}\eta_\beta + u_\beta)\delta_{\alpha\gamma} + (\sqrt{\theta}\eta_\gamma + u_\gamma)\delta_{\alpha\beta} \right\} \\ &= \theta^{3/2}\eta_\alpha\eta_\beta\eta_\gamma + \theta(\eta_\alpha\eta_\beta u_\gamma + \eta_\alpha\eta_\gamma u_\beta + \eta_\beta\eta_\gamma u_\alpha) \\ &\quad + \sqrt{\theta}(\eta_\alpha u_\beta u_\gamma + \eta_\beta u_\alpha u_\gamma + \eta_\gamma u_\alpha u_\beta) + u_\alpha u_\beta u_\gamma \\ &\quad - \sqrt{\theta}(\eta_\alpha \delta_{\beta\gamma} + \eta_\beta \delta_{\alpha\gamma} + \eta_\gamma \delta_{\alpha\beta}) - (u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta}) \end{aligned}$$

CANNOT proof $\mathbf{a}^{(3),\text{eq}}$ currently.

Refer to Eq. (3.61), the explicit Hermite expansion of the Maxwellian f^{eq} is therefore:

$$\begin{aligned} f^{\text{eq}}(\boldsymbol{\xi}) &= \omega(\boldsymbol{\xi}) \sum_{n=0}^{\infty} \frac{1}{n!} \mathbf{a}^{(n),\text{eq}} : \mathcal{H}^{(n)}(\boldsymbol{\xi}) \\ &= \omega(\boldsymbol{\xi}) \left\{ \left(\mathbf{a}^{(1),\text{eq}} : \mathcal{H}^{(1)}(\boldsymbol{\xi}) \right) + \left(\frac{1}{2!} \mathbf{a}^{(2),\text{eq}} : \mathcal{H}^{(2)}(\boldsymbol{\xi}) \right) + \left(\frac{1}{3!} \mathbf{a}^{(3),\text{eq}} : \mathcal{H}^{(3)}(\boldsymbol{\xi}) \right) + \dots \right\} \\ &= \omega(\boldsymbol{\xi}) \rho \left\{ 1 + \boldsymbol{\xi} \cdot \mathbf{u} + \frac{1}{2}(\boldsymbol{\xi}^2 - \delta) : (\mathbf{u}^2 + (\theta - 1)\delta) + \frac{1}{6}(\boldsymbol{\xi}^3 - \boldsymbol{\xi}\delta) : (\mathbf{u}^3 + (\theta - 1)\mathbf{u}\delta) + \dots \right\} \\ &= \omega(\boldsymbol{\xi}) \rho \left\{ 1 + \boldsymbol{\xi} \cdot \mathbf{u} + \frac{1}{2} \{ (\boldsymbol{\xi} \cdot \mathbf{u})^2 - u^2 + (\theta - 1)(\boldsymbol{\xi}^2 - D) \} \right. \\ &\quad \left. + \frac{\boldsymbol{\xi} \cdot \mathbf{u}}{6} \{ (\boldsymbol{\xi} \cdot \mathbf{u})^2 - 3u^2 + 3(\theta - 1)(\boldsymbol{\xi}^2 - D - 2) \} + \dots \right\} \end{aligned}$$

Notice, all the terms proportional to $(\theta - 1)$ vanish for an “isothermal” system in which $\theta = 1$ (Refer to Section 2.1.5 for the meaning of the dimensionless variable θ).

We need to prove the results.

3.2.2 Discretization in Velocity Space

3.2.2.1 Truncation of the Generalized Fourier Series

Sometimes we can represent the integrand as an infinite series but even if we can integrate each term of the series exactly we must still truncate the series and thus approximate the integral.

Owing to the mutual orthogonality of Hermite polynomials, the leading moments of a distribution function up to N th order are preserved by truncation of the higher-order terms in its Hermite expansion, as discussed by Shan et al. [10]. Consequently, a distribution function can be approximated by its projection onto a Hilbert subspace spanned by the first N Hermite polynomials without changing the first N moments, refer to Eq. (3.46), we have

$$f(\mathbf{x}, \boldsymbol{\xi}, t) \approx f_N(\mathbf{x}, \boldsymbol{\xi}, t) = \omega(\boldsymbol{\xi}) \sum_{n=0}^N \frac{1}{n!} \mathbf{a}^{(n)}(\mathbf{x}, t) : \mathcal{H}^{(n)}(\boldsymbol{\xi}) \quad (3.64)$$

Here, up to N th-order, $f_N(\mathbf{x}, \boldsymbol{\xi}, t)$ has exactly the same velocity moments as the original $f(\mathbf{x}, \boldsymbol{\xi}, t)$ does (need more discussions here). This guaranties that a fluid dynamic system can be constructed by a finite set of macroscopic variables (thermo-hydrodynamic moments).

3.2.2.2 Gauss-Hermite Quadrature

Forget Hermite polynomials for a few minutes. The word “quadrature” is a synonym for “numerical integration”.

Gauss Quadrature begins with the specification of an infinite, complete, orthogonal sequence of polynomials in which the domain of the polynomials matches the desired integration interval and the orthogonality condition is consistent with the desired integrand. We choose the Hermite polynomials since they suit our applications well in terms of both the integration interval and desired integrand. (As the reader may have guessed, Gauss Quadrature with Hermite polynomials is “Gauss-Hermite Quadrature”.)

In one dimension, the Gauss-Hermite quadrature is a Gaussian quadrature over the interval $(-\infty, \infty)$ with respect to the weight function of $\omega(x) = e^{-x^2}$ shown in Eq. (3.1). In numerical analysis, Gauss-Hermite quadrature is a form of Gaussian quadrature for approximating the value of integrals of the following kind: $\int_{-\infty}^{+\infty} e^{-x^2} f(x) dx$. In which $f(x)$ are the orthogonal Hermite polynomials and the abscissae of the n -point quadrature are the zeros of $H_n(x)$ as refer to (3.4). In Gauss-Hermite quadrature this integral is approximated by

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x) dx \approx \sum_{i=1}^n w_i f(x_i) \quad (3.65)$$

where n is the number of sample points used. The x_i are the roots (or zeros) of the physicists’ version of the n th order Hermite polynomial $H_n(x)$ as refer to (3.4), and the associated weights w_i are given by [16]

$$w_i = \frac{2^{n-1} n! \sqrt{\pi}}{n^2 \{H_{n-1}(x_i)\}^2} \quad (3.66)$$

with $i = 1, 2, \dots, n$. We will not consider the Gauss-Hermite quadrature of the probabilists’ version of the n th order Hermite polynomial $He_n(x)$ as refer to Eq. (3.3), with weight function $\omega(x) = e^{-x^2/2}$ shown in Eq. (3.1).

However, for our application in LBM, refer to Shan et al. [10], we will consider the Gauss-Hermite quadrature of the probabilists’ version of the n th order Hermite polynomial $\mathcal{H}^{(n)}(x)$ defined in Eq. (3.35) (which is actually identical with $He_n(x)$ shown in Eq. (3.3)), with weight function

$\omega(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$ shown in Eq. (3.34) (which has a scaling factor).

Thus, in Gauss-Hermite quadrature this integral of $\int_{-\infty}^{+\infty} \omega(x) f(x) dx = \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} f(x) dx$ is approximated by [10]

$$\int_{-\infty}^{+\infty} \omega(x) f(x) dx \approx \sum_{i=1}^n w_i f(x_i) \quad (3.67)$$

in which the symbol “ \approx ” means approximation “ \approx ” in general and equal “=” in certain conditions. This is due to the expansion of $f(x)$ based on the Hermite polynomials shown in Eq. (3.45). In practice, though, we will expand $f(x)$ into a finite series of Hermite polynomials as an approximation. So the Gauss-Hermite quadrature approximation improves as we increase the number of terms (equality holds when $n = \infty$). However, as pointed by Shan et al. [10] (A11 in this reference), if the above estimate is said to have an algebraic degree of precision of p , exact equality holds if for any f that is a polynomial of a degree up to p (need more clear and consistent notations for this part about precision).

Again, the corresponding orthogonal polynomials of the Gauss-Hermite quadrature are the Hermite polynomials and the abscissae of the n -point quadrature are the zeros of $\mathcal{H}^{(n)}(x)$. The corresponding weights are [10]:

$$w_i = \frac{n!}{n^2 \{\mathcal{H}^{(n-1)}(x_i)\}^2} \quad (3.68)$$

Table 3.1 gives the numerical values of the abscissae and weights of one-dimensional Gauss-Hermite quadrature up to n th order of Hermite polynomials with $n = 5$, and degree of precision of $p = 9$. For convenience, we shall hereinafter name the quadrature formulae by the convention $E_{D,p}^m$ where D is the dimension of the space, p is the algebraic degree of precision (in one dimension, $p = 2m - 1$), and m is the number of points employed in the quadrature (in one dimension, $m = n$). For example, $E_{1,9}^5$ denotes a degree-9 quadrature formula in 1 dimension employing 5 points, while $E_{2,5}^9$ denotes a degree-5 quadrature formula in 2 dimensions employing 9 points.

We will return to the Gauss-Hermite quadrature in higher dimensions later.

In higher dimensions, no general Gauss quadrature theory is known. Nevertheless, a class of Gauss-Hermite formulae known as “production” formulae can be derived from one-dimensional formulae. For higher dimensions, as discussed in [10, 17], consider a D -dimensional polynomial of degree n , denoted as $\mathbf{p}_n(\boldsymbol{\xi})$, there exists a set of abscissas $\boldsymbol{\xi}_i$ and associated weights, $\{\boldsymbol{\xi}_i, w_i : i = 1, 2, \dots, D\}$, and the Gauss-Hermite quadrature for the integral $\int_{-\infty}^{+\infty} \omega(\boldsymbol{\xi}) \mathbf{p}_n(\boldsymbol{\xi}) d\boldsymbol{\xi} = \frac{1}{(2\pi)^{D/2}} \int_{-\infty}^{+\infty} e^{-\boldsymbol{\xi}^2/2} \mathbf{p}_n(\boldsymbol{\xi}) d\boldsymbol{\xi}$ (n -fold integration) can be approximated as

$$\int \omega(\boldsymbol{\xi}) \mathbf{p}_n(\boldsymbol{\xi}) d\boldsymbol{\xi} = \sum_{i=1}^D w_i \mathbf{p}_n(\boldsymbol{\xi}_i) \quad (3.69)$$

Table 3.1: Abscissae and Weights of One-dimensional Gauss-Hermite Quadrature

Quadrature	x_i	w_i
$E_{1,1}^1$	0	1
$E_{1,3}^2$	± 1	1/2
$E_{1,5}^3$	0 ± 3	2/3 1/6
$E_{1,7}^4$	$\pm\sqrt{3-\sqrt{6}}$ $\pm\sqrt{3+\sqrt{6}}$	$(3+\sqrt{6})/12$ $(3-\sqrt{6})/12$
$E_{1,9}^5$	0 $\pm\sqrt{5-\sqrt{10}}$ $\pm\sqrt{5+\sqrt{10}}$	8/15 $(7+2\sqrt{10})/60$ $(7-2\sqrt{10})/60$

3.2.2.3 Discretization

In order to numerically solve the Boltzmann equation, a discretization of the velocity space is necessary. It consists in keeping only a discrete set of D velocities ξ_i , $i \in [1, 2, \dots, D]$, ensuring the preservation of f_i moments, from the continuum velocity space to the discrete one. To do so, a Gauss-Hermite quadrature is applied.

We first consider the discretization of the Hermite series expansion coefficient $\mathbf{a}^{(n)}$ by using higher dimensional Gauss-Hermite quadrature. Substitute the N th-order truncation of generalized Fourier series (Hermite series) shown in (3.64) into the expansion coefficient $\mathbf{a}^{(n)}$ shown in Eq. (3.46), we have⁶

$$\mathbf{a}^{(n)} = \int f(\xi) \mathcal{H}^{(n)}(\xi) d\xi = \int f_N(\xi) \mathcal{H}^{(n)}(\xi) d\xi \quad (3.70)$$

$$= \int \omega(\xi) \left\{ \frac{f_N(\xi) \mathcal{H}^{(n)}(\xi)}{\omega(\xi)} \right\} d\xi \quad (3.71)$$

Note that the term inside the brackets is an $(N + n)$ -th degree polynomial.

Let M be the highest order of moments that determines the hydrodynamic equations of interest, e.g., $M = 3$ if the momentum equation at the Navier-Stokes level is of concern. As discussed in Section 3.2.1.2, conservation of moments relates to the Hermite series expansion coefficients $\mathbf{a}^{(n)}$, thus consider the leading M ($\leq N$) terms of the expansion coefficients (with truncated Hermite series substituted):

$$\mathbf{a}^{(n)} = \int \omega(\xi) \mathbf{p}(\xi) d\xi, \quad n = 0, 1, 2, \dots, M \quad (3.72)$$

where $\mathbf{p}(\xi)$ is a polynomial of an order $\leq M + N$. Actually it's easy to find that $\omega(\xi) \mathbf{p}(\xi) = f_N(\xi) \mathcal{H}^{(n)}(\xi)$ refer to [10]. Let ξ_i and w_i , $i = 1, 2, \dots, D$, be the abscissas and weights of a degree-

⁶Note that exact equal sign “=” was used here instead of the approximation sign “ \approx ” in the truncation equation (3.64), because up to N th-order, $f_N(\mathbf{x}, \xi, t)$ has exactly the same velocity moments as the original $f(\mathbf{x}, \xi, t)$ does, and the desired order velocity moments can be expressed with $\mathbf{a}^{(n)}$

Q (precision) quadrature rule⁷, the integral of $\mathbf{a}^{(n)}$ can be exactly evaluated using the values of the integrand on a finite set of velocities $\{\xi_i : i = 1, 2, \dots, D\}$, by Eq. (3.69) we have:

$$\mathbf{a}^{(n)} = \int \omega(\xi) \mathbf{p}(\xi) d\xi = \sum_{i=1}^D w_i \mathbf{p}_n(\xi_i) = \sum_{i=1}^D f_i(\xi_i) \mathcal{H}^{(n)}(\xi_i), \quad n = 0, 1, 2, \dots, M \quad (3.73)$$

where

$$f_i(\xi_i) \equiv \frac{w_i \mathbf{p}_n(\xi_i)}{\omega(\xi_i)} = w_i \sum_{n=0}^N \frac{1}{n!} \mathbf{a}^{(n)} : \mathcal{H}^{(n)}(\xi_i) \quad (3.74)$$

Note that $\mathbf{a}^{(n)}$ can be accurately computed from only up to $n = Q - N$. Equation (3.73) defines an isomorphic transform between $\{\mathbf{a}^{(n)} : n = 1, 2, \dots, N\}$ (here let the coefficient expanded to the truncated order, i.e. $Q - N = N$) and $\{f_i(\xi_i) : i = 1, 2, \dots, D\}$ provided that the quadrature is sufficiently accurate, i.e., $Q \geq 2N$, and the distribution function is restricted to the finite-dimensional functional space spanned by the leading Hermite polynomials, i.e., that defined by Eq. (3.64) [17]. Also to be noted is that, $Q - N$ and N , whichever is smaller, determines the order of moments that can be represented by the discrete velocities and hence, it is optimum to use a quadrature with $Q - N = N \Rightarrow Q = 2N$.

Equation (3.73) holds if and only if ξ_i are the abscissas of a Gauss-Hermite quadrature of a degree of precision $Q \geq M + N$ and w_i the corresponding weights. It can now be concluded that the sufficient conditions for the BGK system to have correct hydrodynamic equations are [18]:

- (1) The equilibrium distribution retains the necessary moments.
- (2) The discrete velocity set allows the moments to be exactly evaluated using finite function values.

Quantitatively, these two conditions are:

$$M \leq N \quad \text{and} \quad M + N \leq Q \quad (3.75)$$

Since Q is finite for any finite set of velocities and $N \leq Q$, N must be finite, i.e., the equilibrium distribution in BGK is the sum of a *finite* Hermite series of an order which is smaller than the degree of the quadrature.

The requirements for the momentum equation to be fully **Galilean invariant**⁸ at the Navier-Stokes level are immediately clear. Since $M = 3$ in this case, we have $N \geq 3$ and $Q \geq 6$. Namely f^{eq} must retain all Hermite terms up to the third order and the discrete velocity set must form a 6th-order accurate Hermite quadrature.

The analysis above can be applied to the case of energy equation where full recovery of the Navier-Stokes energy equation requires $N \geq M \geq 4$, and $Q \geq 8$. Using a third-order expansion ($N = 3$), or a velocity set that only supports third-order moments ($6 \leq Q < 8$) could yield otherwise correct thermal BGK models with a velocity-dependent thermal diffusivity (not Galilean invariant).

⁷Here, for an exact approximation, the highest order of the polynomial $\mathbf{p}(\xi)$, $M + N$ should be less or equal than Q , and we can choose M according $M + N = Q$ or $M = Q - N$, as discussed by Shan et al. [17].

⁸Galilean invariance means that the model must not be affected by a Galilean transformation. A Galilean transformation is a change of reference frame from one coordinate system to another moving with a constant velocity relative to the original. Everything in classical physics is Galilean invariant so all physical models should also be Galilean invariant in order to be correct.

3.2.3 Discretization of Space and Time

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Chapter 4 The Chapman-Enskog Anylysis

4.1 Perturbation Method

A response variable q may be represented by the perturbed form:

$$q = q_0 + \epsilon q_1 + \epsilon^2 q_2 + \dots \quad (4.1)$$

where the term $q_0(x, t)$ corresponds to the response with all nonlinear terms set to zero, or the equilibrium state.

For the variable x and t , since different physical phenomenon happens on different space and time scales, thus x and t may be expressed as:

$$x = x(x_0, x_1, x_2, \dots); t = t(t_0, t_1, t_2, \dots) \quad (4.2)$$

where $x_j = \epsilon^j x_0$, $x_0 \approx x$ and $t_j = \epsilon^j t_0$, $t_0 \approx t$.

Take the time scale t as an example. As t_0 changes by 1 unit, t_j changes by only ϵ^j unit. Thus, t_0 is referred as the fast time variable, and t_j as the slow time variables. The constant $\epsilon < 1$ so t_k varies faster than t_{k+1} , which is faster than t_{k+2} , etc. To help grasp the concept of different time scales one might for sake of analogy consider seconds as the t_0 unit, minutes as the t_1 unit, hours as the t_2 unit, etc.

The corresponding series formulas for space and time derivatives of q as shown below.

Applying the chain rule yields the first derivative operator for time:

$$\frac{d}{dt} = \frac{\partial}{\partial t_0} \frac{\partial t_0}{\partial t} + \frac{\partial}{\partial t_1} \frac{\partial t_1}{\partial t} + \dots = \frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \dots \quad (4.3)$$

The second derivative operator for time is (will not be used in this document):

$$\begin{aligned} \frac{d^2}{dt^2} &= \frac{d}{dt} \left(\frac{d}{dt} \right) = \left(\frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \dots \right) \left(\frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \dots \right) \\ &= \frac{\partial^2}{\partial t_0^2} + \epsilon \left(2 \frac{\partial^2}{\partial t_0 \partial t_1} \right) + \epsilon^2 \left(2 \frac{\partial^2}{\partial t_0 \partial t_2} + \frac{\partial^2}{\partial t_1^2} \right) + \dots \end{aligned} \quad (4.4)$$

Same for first derivative operator for space:

$$\frac{d}{dx} = \frac{\partial}{\partial x_0} \frac{\partial x_0}{\partial x} + \frac{\partial}{\partial x_1} \frac{\partial x_1}{\partial x} + \dots = \frac{\partial}{\partial x_0} + \epsilon \frac{\partial}{\partial x_1} + \dots \quad (4.5)$$

If the variable varies very slowly in x_0 and t_0 scale (focus on mesoscopic scale or the free path of particles, not the characteristic length of the macroscopic problem), we get the following multi-scale expressions for the Chapman-Enskog expansion [1, 2]:

$$f_i = f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} + \mathcal{O}(\epsilon^3) \quad (4.6a)$$

$$\frac{\partial}{\partial t} = \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \mathcal{O}(\epsilon^3) \quad (4.6b)$$

$$\frac{\partial}{\partial \mathbf{r}} = \epsilon \frac{\partial}{\partial \mathbf{r}_1} + \mathcal{O}(\epsilon^2) \quad (4.6c)$$

in which, $\frac{\partial}{\partial \mathbf{r}} = \nabla = \mathbf{e}_x \frac{\partial}{\partial x} + \mathbf{e}_y \frac{\partial}{\partial y} + \mathbf{e}_z \frac{\partial}{\partial z} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$ [3].

If want to use a more consistent notation, we use $\frac{\partial}{\partial t_1} = \partial_{t_1} = \partial_t^{(1)}$, $\frac{\partial}{\partial t_2} = \partial_{t_2} = \partial_t^{(2)}$ and $\frac{\partial}{\partial \mathbf{r}_1} = \partial_{\mathbf{r}_1} = \partial_{\mathbf{r}}^{(1)}$ (or $\nabla_{\mathbf{r}_1} = \nabla_{\mathbf{r}}^{(1)}$). The multi-scale form expressed in Eq. (4.6) has an alternative form:

$$\begin{aligned} f_i &= f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} + \mathcal{O}(\epsilon^3) \\ \partial_t &= \epsilon \partial_t^{(1)} + \epsilon^2 \partial_t^{(2)} + \mathcal{O}(\epsilon^3) \end{aligned} \quad (4.7a)$$

$$\partial_{\mathbf{r}} = \epsilon \partial_{\mathbf{r}}^{(1)} + \mathcal{O}(\epsilon^2) \quad \text{or} \quad \nabla_{\mathbf{r}} = \epsilon \nabla_{\mathbf{r}}^{(1)} + \mathcal{O}(\epsilon^2) \quad (4.7b)$$

Where ϵ is a small parameter proportional to the Knudsen number. Note that space derivatives (not gradient) are analyzed at a single scale.

Or from [4], the LB dynamics is developed into a truncated Taylor series in space and time, up to second-order accuracy. Furthermore, to separate physical phenomena happening at different scales, the particle populations are expanded into a power-law series with respect to a small parameter $\epsilon \ll 1$, $f_i = \sum_{k=0}^{\infty} \epsilon^k f_i^{(k)}$. The two first terms, of order $\mathcal{O}(\epsilon^0)$ and order $\mathcal{O}(\epsilon^1)$, are sufficient to recover asymptotically the dynamics of the Navier-Stokes equation.

4.2 Taylor Expansion

Let f be an infinitely differentiable function in some open neighborhood around $(x, y) = (a, b)$, then:

$$\begin{aligned} f(x, y) &= f(a, b) + f_x(a, b)(x - a) + f_y(a, b)(y - b) \\ &+ \frac{1}{2!} \{ f_{xx}(a, b)(x - a)^2 + 2f_{xy}(a, b)(x - a)(y - b) \\ &+ f_{yy}(a, b)(y - b)^2 \} + \dots \end{aligned} \quad (4.8)$$

By discretizing the Boltzmann-BGK model, the lattice Boltzmann equation (LBE) can be derived:

$$\boxed{f_i(\mathbf{r} + \mathbf{c}_i \delta_t, t + \delta_t) = f_i(\mathbf{r}, t) - \frac{1}{\tau} \{ f_i(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r}, t) \}} \quad (4.9)$$

Note that in Eq. (4.9), τ has no unit, not even lattice time unit. However, if use Eq. (4.10) as follows as adopted in reference [2], then τ has a lattice time unit.

$$f_i(\mathbf{r} + \mathbf{c}_i \delta_t, t + \delta_t) = f_i(\mathbf{r}, t) - \frac{\delta_t}{\tau} \{ f_i(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r}, t) \} \quad (4.10)$$

Note that for the following Boltzmann-BGK equation indicates that τ has a lattice time unit follow-

ing the second form in Eq. (4.10). However, to simplify the derivation process, we will not use this form, we use the first form in Eq. (4.9) with τ being the dimensionless relaxation time.

The discretized lattice Boltzmann-BGK equation shown in Eq. (4.9) can be derived from the Boltzmann-BGK equation shown in Eq. (4.11).

$$\boxed{\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau}(f - f^{\text{eq}})} \quad (4.11)$$

Throughout the rest of this section we shall assume that velocity space is discretized, which means that will use the discretized Boltzmann-BGK equation in Eq. (4.9).

Do the Taylor expansion for space and time for $f_i(\mathbf{r} + \mathbf{c}_i \delta_t, t + \delta_t)$ in Eq. (4.9), we get:

$$f_i(\mathbf{r} + \mathbf{c}_i \delta_t, t + \delta_t) = f_i(\mathbf{r}, t) + \frac{\partial}{\partial t} f_i(\mathbf{r}, t) \delta_t + \frac{\partial}{\partial \mathbf{r}} \cdot \{f_i(\mathbf{r}, t) \mathbf{c}_i \delta_t\} + \dots \quad (4.12)$$

Substitute the Taylor expansion of $f_i(\mathbf{r} + \mathbf{c}_i \delta_t, t + \delta_t)$ into Eq. (4.9), we can obtain that

$$\delta_t \left(\frac{\partial}{\partial t} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}} \right) f_i(\mathbf{r}, t) + \frac{\delta_t^2}{2} \left(\frac{\partial}{\partial t} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}} \right)^2 f_i(\mathbf{r}, t) + \frac{1}{\tau} \{f_i(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r}, t)\} + \mathcal{O}(\delta_t^3) = 0 \quad (4.13)$$

or in index notation:

$$\delta_t (\partial_t + c_{i\alpha} \partial_\alpha) f_i(\mathbf{r}, t) + \frac{\delta_t^2}{2} (\partial_t + c_{i\alpha} \partial_\alpha)^2 f_i(\mathbf{r}, t) + \frac{1}{\tau} \{f_i(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r}, t)\} + \mathcal{O}(\delta_t^3) = 0 \quad (4.14)$$

If there is no truncation in the Taylor expansion, we have [5]:

$$\left\{ \sum_{n=1}^{\infty} \frac{\delta_t^n}{n!} \left(\frac{\partial}{\partial t} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}} \right)^n \right\} f_i(\mathbf{r}, t) = -\frac{1}{\tau} \{f_i(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r}, t)\} \quad (4.15)$$

or in index notation [2]:

$$\left\{ \sum_{n=1}^{\infty} \frac{\delta_t^n}{n!} (\partial_t + c_{i\alpha} \partial_\alpha)^n \right\} f_i(\mathbf{r}, t) = -\frac{1}{\tau} \{f_i(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r}, t)\} \quad (4.16)$$

4.3 Recombination

4.3.1 Mesoscopic Mass and Momentum Conservation

4.3.1.1 Multi-Scale Analysis

Substitute the multi-scale expressions from Eq. (4.6), we have:

$$\begin{aligned} \delta_t \left(\epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \epsilon \mathbf{c}_i \cdot \nabla_{\mathbf{r}_1} \right) \left(f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} \right) + \\ \frac{\delta_t^2}{2} \left(\epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \epsilon \mathbf{c}_i \cdot \nabla_{\mathbf{r}_1} \right)^2 \left(f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} \right) + \\ \frac{1}{\tau} \left(f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} - f_i^{\text{eq}} \right) + \mathcal{O}(\delta_t^3) = 0 \end{aligned} \quad (4.17)$$

or in index notation:

$$\begin{aligned}
& \delta_t \left(\epsilon \partial_t^{(1)} + \epsilon^2 \partial_t^{(2)} + \epsilon c_{i\alpha} \partial_\alpha^{(1)} \right) \left(f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} \right) + \\
& \quad \frac{\delta_t^2}{2} \left(\epsilon \partial_t^{(1)} + \epsilon^2 \partial_t^{(2)} + \epsilon c_{i\alpha} \partial_\alpha^{(1)} \right)^2 \left(f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} \right) + \\
& \quad \frac{1}{\tau} \left(f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} - f_i^{\text{eq}} \right) + \mathcal{O}(\delta_t^3) = 0 \quad (4.18)
\end{aligned}$$

According to the formulations at different orders of ϵ , we have:

$$\begin{cases}
\mathcal{O}(\epsilon^0) : & \frac{1}{\tau} (f_i^{(0)} - f_i^{\text{eq}}) = 0 \\
\mathcal{O}(\epsilon^1) : & \left(\frac{\partial}{\partial t_1} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}_1} \right) f_i^{(0)} + \frac{1}{\tau \delta_t} f_i^{(1)} = 0 \\
\mathcal{O}(\epsilon^2) : & \frac{\partial f_i^{(0)}}{\partial t_2} + \left(\frac{\partial}{\partial t_1} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}_1} \right) f_i^{(1)} + \frac{\delta_t}{2} \left(\frac{\partial}{\partial t_1} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}_1} \right)^2 f_i^{(0)} + \frac{1}{\tau} \delta_t f_i^{(2)} = 0
\end{cases} \quad (4.19)$$

or in index notation:

$$\begin{cases}
\mathcal{O}(\epsilon^0) : & \frac{1}{\tau} (f_i^{(0)} - f_i^{\text{eq}}) = 0 \\
\mathcal{O}(\epsilon^1) : & \left(\partial_t^{(1)} + c_{i\alpha} \partial_\alpha^{(1)} \right) f_i^{(0)} + \frac{1}{\tau \delta_t} f_i^{(1)} = 0 \\
\mathcal{O}(\epsilon^2) : & \partial_t^{(2)} f_i^{(0)} + \left(\partial_t^{(1)} + c_{i\alpha} \partial_\alpha^{(1)} \right) f_i^{(1)} + \frac{\delta_t}{2} \left(\partial_t^{(1)} + c_{i\alpha} \partial_\alpha^{(1)} \right)^2 f_i^{(0)} + \frac{1}{\tau \delta_t} f_i^{(2)} = 0
\end{cases} \quad (4.20)$$

Note that from Eq. (4.19), it is concluded that the collision term Ω_i does not contain constant contributions with respect to the parameter ϵ : $\Omega_i^{(0)} = 0$ [6]. Thus if we need to separate the collision term to different scales, the collision term should be expanded starting from the $\mathcal{O}(\epsilon^1)$ term:

$$\Omega_i = -\frac{1}{\tau} \{ f_i(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r}, t) \} = \epsilon \Omega_i^{(1)} + \epsilon^2 \Omega_i^{(2)} + \mathcal{O}(\epsilon^3)$$

Combine $\mathcal{O}(\epsilon^1)$ and $\mathcal{O}(\epsilon^2)$ from Eq. (4.19), an assume τ is constant with (\mathbf{r}, t) , we get:

$$\mathcal{O}(\epsilon^2) : \quad \frac{\partial f_i^{(0)}}{\partial t_2} + \left(1 - \frac{1}{2\tau} \right) \left(\frac{\partial}{\partial t_1} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}_1} \right) f_i^{(1)} + \frac{1}{\tau \delta_t} f_i^{(2)} = 0$$

or in index notation, combine $\mathcal{O}(\epsilon^1)$ and $\mathcal{O}(\epsilon^2)$ from Eq. (4.20), we have:

$$\mathcal{O}(\epsilon^2) : \quad \partial_t^{(2)} f_i^{(0)} + \left(1 - \frac{1}{2\tau} \right) \left(\partial_t^{(1)} + c_{i\alpha} \partial_\alpha^{(1)} \right) f_i^{(1)} + \frac{1}{\tau \delta_t} f_i^{(2)} = 0$$

Thus, we obtain the updated version of the scale order analysis for Eq. (4.19), as

$$\begin{cases}
\mathcal{O}(\epsilon^0) : & \frac{1}{\tau} (f_i^{(0)} - f_i^{\text{eq}}) = 0 \\
\mathcal{O}(\epsilon^1) : & \left(\frac{\partial}{\partial t_1} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}_1} \right) f_i^{(0)} + \frac{1}{\tau \delta_t} f_i^{(1)} = 0 \\
\mathcal{O}(\epsilon^2) : & \frac{\partial f_i^{(0)}}{\partial t_2} + \left(1 - \frac{1}{2\tau} \right) \left(\frac{\partial}{\partial t_1} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}_1} \right) f_i^{(1)} + \frac{1}{\tau \delta_t} f_i^{(2)} = 0
\end{cases} \quad (4.21)$$

or in index notation:

$$\begin{cases} \mathcal{O}(\epsilon^0) : & \frac{1}{\tau} (f_i^{(0)} - f_i^{\text{eq}}) = 0 \\ \mathcal{O}(\epsilon^1) : & \left(\partial_t^{(1)} + c_{i\alpha} \partial_\alpha^{(1)} \right) f_i^{(0)} + \frac{1}{\tau \delta_t} f_i^{(1)} = 0 \\ \mathcal{O}(\epsilon^2) : & \partial_t^{(2)} f_i^{(0)} + \left(1 - \frac{1}{2\tau} \right) \left(\partial_t^{(1)} + c_{i\alpha} \partial_\alpha^{(1)} \right) f_i^{(1)} + \frac{1}{\tau \delta_t} f_i^{(2)} = 0 \end{cases} \quad (4.22)$$

From $\mathcal{O}(\epsilon^0)$,

$$f_i^{(0)} = f_i^{\text{eq}} \quad (4.23)$$

From $\mathcal{O}(\epsilon^1)$, we can obtain the relation between the first-order distribution functions $f_i^{(1)}$ and the equilibrium distribution functions f_i^{eq} , as:

$$f_i^{(1)} = -\tau \delta_t \left(\frac{\partial}{\partial t_1} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}_1} \right) f_i^{\text{eq}} \quad (4.24)$$

or in index notation:

$$f_i^{(1)} = -\tau \delta_t \left(\partial_t^{(1)} + c_{i\alpha} \partial_\alpha^{(1)} \right) f_i^{\text{eq}} \quad (4.25)$$

4.3.1.2 Mesoscopic Conservation Rules

According the mass conservation, the mass of the current state equals to the mass of the equilibrium state of a system, thus

$$\begin{aligned} \rho(\mathbf{r}, t) &= \sum_i f_i(\mathbf{r}, t) \\ &= \sum_i f_i^{(0)}(\mathbf{r}, t) + \epsilon \sum_i f_i^{(1)}(\mathbf{r}, t) + \epsilon^2 \sum_i f_i^{(2)}(\mathbf{r}, t) \\ &= \sum_i f_i^{\text{eq}}(\mathbf{r}, t) \end{aligned} \quad (4.26)$$

So we can derive that:

$$\sum_i f_i^{(1)}(\mathbf{r}, t) = \sum_i f_i^{(2)}(\mathbf{r}, t) = 0 \quad (4.27)$$

Also, from the momentum conservation, we have

$$\begin{aligned} \rho(\mathbf{r}, t) \mathbf{u}(\mathbf{r}, t) &= \sum_i \mathbf{c}_i f_i(\mathbf{r}, t) \\ &= \sum_i \mathbf{c}_i f_i^{(0)}(\mathbf{r}, t) + \epsilon \sum_i \mathbf{c}_i f_i^{(1)}(\mathbf{r}, t) + \epsilon^2 \sum_i \mathbf{c}_i f_i^{(2)}(\mathbf{r}, t) \\ &= \sum_i \mathbf{c}_i f_i^{\text{eq}}(\mathbf{r}, t) \end{aligned} \quad (4.28)$$

or in index notation $\rho u_\alpha = \sum_i c_\alpha f_i^{(0)} = \sum_i c_\alpha f_i^{\text{eq}}$.

So we can derive that:

$$\sum_i \mathbf{c}_i f_i^{(1)}(\mathbf{r}, t) = \sum_i \mathbf{c}_i f_i^{(2)}(\mathbf{r}, t) = 0 \quad (4.29)$$

4.3.1.3 Mass Conservation

Get the zeroth order moment (take summation) of $\mathcal{O}(\epsilon^1)$ and $\mathcal{O}(\epsilon^2)$ from Eq. (4.21), apply the mesoscopic conservation rules in Section 4.3.1.2 we get:

$$\begin{cases} \mathcal{O}(\epsilon^1) : & \frac{\partial}{\partial t_1} \sum_i f_i^{(0)} + \frac{\partial}{\partial \mathbf{r}_1} \cdot (\sum_i \mathbf{c}_i f_i^{(0)}) = 0 \\ \mathcal{O}(\epsilon^2) : & \frac{\partial}{\partial t_2} \sum_i f_i^{(0)} = 0 \end{cases} \quad (4.30)$$

or in index notation from Eq. (4.22) and apply the mesoscopic conservation rules in Section 4.3.1.2:

$$\begin{cases} \mathcal{O}(\epsilon^1) : & \partial_t^{(1)} \sum_i f_i^{(0)} + \partial_\alpha^{(1)} (\sum_i c_{i\alpha} f_i^{(0)}) = 0 \\ \mathcal{O}(\epsilon^2) : & \partial_t^{(2)} \sum_i f_i^{(0)} = 0 \end{cases} \quad (4.31)$$

From the mesoscopic conservation rules in Section 4.3.1.2, we have:

$$\begin{cases} \mathcal{O}(\epsilon^1) : & \frac{\partial}{\partial t_1} \rho + \frac{\partial}{\partial \mathbf{r}_1} \cdot (\rho \mathbf{u}) = 0 \\ \mathcal{O}(\epsilon^2) : & \frac{\partial}{\partial t_2} \rho = 0 \end{cases} \quad (4.32)$$

or in index notation:

$$\begin{cases} \mathcal{O}(\epsilon^1) : & \partial_t^{(1)} \rho + \partial_\alpha^{(1)} (\rho u_\alpha) = 0 \\ \mathcal{O}(\epsilon^2) : & \partial_t^{(2)} \rho = 0 \end{cases} \quad (4.33)$$

We can see that [2] the continuity equation is exact already at $\mathcal{O}(\epsilon^1)$ so we might have expected that the $\mathcal{O}(\epsilon^2)$ correction is zero. Then we can derive:

$$\left(\epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} \right) \rho + \epsilon \nabla_{\mathbf{r}_1} \cdot (\rho \mathbf{u}) = 0 \quad (4.34)$$

or in index notation:

$$\left(\epsilon \partial_t^{(1)} + \epsilon^2 \partial_t^{(2)} \right) \rho + \epsilon \partial_\alpha^{(1)} (\rho u_\alpha) = 0 \quad (4.35)$$

Refer to the multi-scale expressions from Eq. (4.6), we recover the mass conservation equation, which is the same as Eq. (1.9):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (4.36)$$

4.3.1.4 Momentum Conservation

Get the first order moment (i.e. multiplying by \mathbf{c}_i and then summing over i) of $\mathcal{O}(\epsilon^1)$ and $\mathcal{O}(\epsilon^2)$ from Eq. (4.21), and apply the mesoscopic conservation rules in Section 4.3.1.2, we get:

$$\begin{cases} \mathcal{O}(\epsilon^1) : & \frac{\partial}{\partial t_1} \sum_i \mathbf{c}_i f_i^{(0)} + \frac{\partial}{\partial \mathbf{r}_1} \cdot (\sum_i \mathbf{c}_i \mathbf{c}_i f_i^{(0)}) = 0 \\ \mathcal{O}(\epsilon^2) : & \frac{\partial}{\partial t_2} \sum_i \mathbf{c}_i f_i^{(0)} + \left(1 - \frac{1}{2\tau} \right) \frac{\partial}{\partial \mathbf{r}_1} \cdot (\sum_i \mathbf{c}_i \mathbf{c}_i f_i^{(1)}) = 0 \end{cases} \quad (4.37)$$

In index notation, get the first order moment (i.e. multiplying by $c_{i\alpha}$ and then summing over i) of $\mathcal{O}(\epsilon^1)$ and $\mathcal{O}(\epsilon^2)$ from Eq. (4.22). When using Eq. (4.22), we need to mention that from here and in the following, we will roll up the index α in $c_{i\alpha}\partial_\alpha^{(1)}$ term to β with $c_{i\beta}\partial_\beta^{(1)}$ term in order to reserve the lowest index α to the time derivative $\partial_t^{(1)}$, $\partial_t^{(2)}$ and finally ∂_t term. We will roll up the index α to γ when get the second order moment later. Then apply the mesoscopic conservation rules in Section 4.3.1.2, we get:

$$\begin{cases} \mathcal{O}(\epsilon^1): & \partial_t^{(1)} \sum_i c_{i\alpha} f_i^{(0)} + \partial_\beta^{(1)} \left(\sum_i c_{i\alpha} c_{i\beta} f_i^{(0)} \right) = 0 \\ \mathcal{O}(\epsilon^2): & \partial_t^{(2)} \sum_i c_{i\alpha} f_i^{(0)} + \left(1 - \frac{1}{2\tau} \right) \partial_\beta^{(1)} \left(\sum_i c_{i\alpha} c_{i\beta} f_i^{(1)} \right) = 0 \end{cases} \quad (4.38)$$

We can see that the $\mathcal{O}(\epsilon^2)$ correction to the Euler momentum equation is non-zero, though given by the as of yet unknown moment $\mathbf{\Pi}^{(1)} = \sum_i \mathbf{c}_i \mathbf{c}_i f_i^{(1)}$ or expressed as $\Pi_{\alpha\beta}^{(1)} = \sum_i c_{i\alpha} c_{i\beta} f_i^{(1)}$ in index notation, as will be discussed later.

To the first order of ϵ , the distribution function f_i is approximated by:

$$f_i = f_i^{(0)} + \epsilon f_i^{(1)} + \mathcal{O}(\epsilon^2) \quad (4.39)$$

We can define the non-equilibrium distribution functions (non-equilibrium populations [5]), as:

$$f_i^{\text{neq}} = f_i - f_i^{\text{eq}} = \epsilon f_i^{(1)} \Rightarrow f_i = f_i^{\text{eq}} + f_i^{\text{neq}} \quad (4.40)$$

From the definition and according to the conservation laws:

$$\sum_i f_i^{\text{neq}} = 0 \quad (4.41)$$

$$\sum_i \mathbf{c}_i f_i^{\text{neq}} = 0 \quad (4.42)$$

We can then define the second-order moments $\mathbf{\Pi}$ of the distribution functions:

$$\begin{aligned} \mathbf{\Pi} &= \sum_i \mathbf{c}_i \mathbf{c}_i f_i = \sum_i \sum_j \mathbf{c}_i \mathbf{c}_j (f_i^{\text{eq}} + f_i^{\text{neq}}) \\ &= \sum_i \mathbf{c}_i \mathbf{c}_i f_i^{\text{eq}} + \sum_i \mathbf{c}_i \mathbf{c}_i f_i^{\text{neq}} \\ &= \mathbf{\Pi}^{\text{eq}} + \mathbf{\Pi}^{\text{neq}} \end{aligned} \quad (4.43)$$

Similar to the definition of the perturbation populations, the perturbation moment (multi-scale expansion) can also be defined:

$$\mathbf{\Pi} = \mathbf{\Pi}^{(0)} + \epsilon \mathbf{\Pi}^{(1)} + \mathcal{O}(\epsilon^2) \quad (4.44)$$

in which, $\mathbf{\Pi}^{(0)} = \sum_i \mathbf{c}_i \mathbf{c}_i f_i^{(0)}$ and $\mathbf{\Pi}^{(1)} = \sum_i \mathbf{c}_i \mathbf{c}_i f_i^{(1)}$. Take the second order moment of $\mathcal{O}(\epsilon^1)$ from Eq. (4.21), we get $\mathbf{\Pi}^{\text{eq}} = \mathbf{\Pi}^{(0)}$, then it's obvious that

$$\mathbf{\Pi}^{\text{neq}} = \epsilon \mathbf{\Pi}^{(1)} \quad (4.45)$$

If expressed in index notation, refer the macroscopic-moments (2.49): $\Pi_{\alpha\beta}^{\text{eq}} = \Gamma_{\alpha\beta}^{\text{eq}} = \sum_i c_{i\alpha} c_{i\beta} f_i^{\text{eq}}$ and $\Pi_{\alpha\beta}^{\text{neq}} = \sum_i c_{i\alpha} c_{i\beta} f_i^{\text{neq}} = \epsilon \Pi_{\alpha\beta}^{(1)} = \epsilon \sum_i c_{i\alpha} c_{i\beta} f_i^{(1)}$.

From the mesoscopic conservation rules in Section 4.3.1.2, we know that $\sum_i \mathbf{c}_i f_i^{(0)} = \rho \mathbf{u}$ or in index notation $\sum_i c_{i\alpha} f_i^{(0)} = \rho u_\alpha$. Combine $\mathcal{O}(\epsilon^1)$ and $\mathcal{O}(\epsilon^2)$, and refer to the multi-scale expressions from Eq. (4.6), we have:

$$\begin{aligned} & \left(\epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} \right) \sum_i \mathbf{c}_i f_i^{(0)} + \epsilon \nabla_{\mathbf{r}_1} \cdot \left(\sum_i \mathbf{c}_i \mathbf{c}_i f_i^{(0)} \right) + \epsilon^2 \left(1 - \frac{1}{2\tau} \right) \nabla_{\mathbf{r}_1} \cdot \left(\sum_i \mathbf{c}_i \mathbf{c}_i f_i^{(1)} \right) \\ &= \left(\epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} \right) \rho \mathbf{u} + \epsilon \nabla_{\mathbf{r}_1} \cdot \mathbf{\Pi}^{(0)} + \epsilon^2 \left(1 - \frac{1}{2\tau} \right) \nabla_{\mathbf{r}_1} \cdot \mathbf{\Pi}^{(1)} \\ &= \frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla_{\mathbf{r}} \cdot \mathbf{\Pi}^{(0)} + \epsilon \left(1 - \frac{1}{2\tau} \right) \nabla_{\mathbf{r}} \cdot \mathbf{\Pi}^{(1)} = 0 \end{aligned} \quad (4.46)$$

or in index notation:

$$\begin{aligned} & \left(\epsilon \partial_t^{(1)} + \epsilon^2 \partial_t^{(2)} \right) \sum_i c_{i\alpha} f_i^{(0)} + \epsilon \partial_\beta^{(1)} \left(\sum_i c_{i\alpha} c_{i\beta} f_i^{(0)} \right) + \epsilon^2 \left(1 - \frac{1}{2\tau} \right) \partial_\beta^{(1)} \left(\sum_i c_{i\alpha} c_{i\beta} f_i^{(1)} \right) \\ &= \left(\epsilon \partial_t^{(1)} + \epsilon^2 \partial_t^{(2)} \right) (\rho u_\alpha) + \epsilon \partial_\beta^{(1)} \Pi_{\alpha\beta}^{(0)} + \epsilon^2 \left(1 - \frac{1}{2\tau} \right) \partial_\beta^{(1)} \Pi_{\alpha\beta}^{(1)} \\ &= \partial_t(\rho u_\alpha) + \partial_\beta \Pi_{\alpha\beta}^{(0)} + \epsilon \left(1 - \frac{1}{2\tau} \right) \partial_\beta \Pi_{\alpha\beta}^{(1)} = 0 \end{aligned} \quad (4.47)$$

Thereafter, we obtain the macro-scale form [1][5]:

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot \mathbf{M} = 0 \quad (4.48)$$

or in index notation:

$$\partial_t(\rho u_\alpha) + \partial_\beta M_{\alpha\beta} = 0 \quad (4.49)$$

in which, \mathbf{M} is the momentum flux tensor, with components as:

$$\mathbf{M} = \sum_i \left\{ \mathbf{c}_i \mathbf{c}_i \left(f_i^{(0)} + \epsilon \left(1 - \frac{1}{2\tau} \right) f_i^{(1)} \right) \right\} = \mathbf{\Pi}^{(0)} + \epsilon \left(1 - \frac{1}{2\tau} \right) \mathbf{\Pi}^{(1)} \quad (4.50)$$

or in index notation

$$M_{\alpha\beta} = \sum_i \left\{ c_{i\alpha} c_{i\beta} \left(f_i^{(0)} + \epsilon \left(1 - \frac{1}{2\tau} \right) f_i^{(1)} \right) \right\} = \Pi_{\alpha\beta}^{(0)} + \epsilon \left(1 - \frac{1}{2\tau} \right) \Pi_{\alpha\beta}^{(1)} \quad (4.51)$$

From the definition of the non-equilibrium distribution functions in Eq. (4.40), the components of the momentum flux tensor \mathbf{M} will be updated as:

$$\mathbf{M} = \sum_i \left\{ \mathbf{c}_i \mathbf{c}_i \left(f_i^{\text{eq}} + \left(1 - \frac{1}{2\tau} \right) f_i^{\text{neq}} \right) \right\} = \mathbf{\Pi}^{\text{eq}} + \left(1 - \frac{1}{2\tau} \right) \mathbf{\Pi}^{\text{neq}} \quad (4.52)$$

or in index notation:

$$M_{\alpha\beta} = \sum_i \left\{ c_{i\alpha} c_{i\beta} \left(f_i^{\text{eq}} + \left(1 - \frac{1}{2\tau} \right) f_i^{\text{neq}} \right) \right\} = \Pi_{\alpha\beta}^{\text{eq}} + \left(1 - \frac{1}{2\tau} \right) \Pi_{\alpha\beta}^{\text{neq}} \quad (4.53)$$

Up to now, the governing conservation equations of mass and momentum in LBM are [1]:

$$\begin{cases} \frac{\partial}{\partial t} \left(\sum_i f_i^{\text{eq}} \right) + \nabla \cdot \left(\sum_i \mathbf{c}_i f_i^{\text{eq}} \right) = 0 \\ \frac{\partial}{\partial t} \left(\sum_i \mathbf{c}_i f_i^{\text{eq}} \right) + \nabla \cdot \left\{ \sum_i \mathbf{c}_i \mathbf{c}_i f_i^{\text{eq}} + \left(1 - \frac{1}{2\tau} \right) \sum_i \mathbf{c}_i \mathbf{c}_i f_i^{\text{neq}} \right\} = 0 \end{cases} \quad (4.54)$$

or in index notation:

$$\begin{cases} \partial_t \left(\sum_i f_i^{\text{eq}} \right) + \partial_\alpha \left(\sum_i c_{i\alpha} f_i^{\text{eq}} \right) = 0 \\ \partial_t \left(\sum_i c_{i\alpha} f_i^{\text{eq}} \right) + \partial_\beta \left\{ \sum_i c_{i\alpha} c_{i\beta} f_i^{\text{eq}} + \left(1 - \frac{1}{2\tau} \right) \sum_i c_{i\alpha} c_{i\beta} f_i^{\text{neq}} \right\} = 0 \end{cases} \quad (4.55)$$

And according to mesoscopic conservation rules, the conservation equations can be described in the following form:

$$\begin{cases} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \\ \frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot \left\{ \mathbf{\Pi}^{\text{eq}} + \left(1 - \frac{1}{2\tau} \right) \mathbf{\Pi}^{\text{neq}} \right\} = 0 \end{cases} \quad (4.56)$$

or in index notation:

$$\begin{cases} \partial_t \rho + \partial_\alpha (\rho u_\alpha) = 0 \\ \partial_t (\rho u_\alpha) + \partial_\beta \left\{ \Pi_{\alpha\beta}^{\text{eq}} + \left(1 - \frac{1}{2\tau} \right) \Pi_{\alpha\beta}^{\text{neq}} \right\} = 0 \end{cases} \quad (4.57)$$

For Chapman-Enskog multiscale analysis, need to include the procedures of a basic paper: *Chen, Shiyi, and Gary D. Doolen. Lattice Boltzmann method for fluid flows. Annual review of fluid mechanics. 1998. 30: 329-364.*

4.3.2 Macroscopic Mass and Momentum Conservation

4.3.2.1 The Momentum Flux Tensor

The momentum flux tensor comes from the momentum equation of Navier-Stokes equations:

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot \mathbf{P} = 0 \quad (4.58)$$

Or, using indices (where it is easier to see that \mathbf{P} is a rank-2 tensor):

$$\frac{\partial (\rho u_\alpha)}{\partial t} + \frac{\partial P_{\alpha\beta}}{\partial \beta} = 0 \quad (4.59)$$

We can split this tensor into three components:

- (1) advection of α -momentum in the β -direction: $(\rho u_\alpha) u_\beta$
- (2) pressure: $p \delta_{\alpha\beta}$
- (3) the viscous stress tensor [7], or deviatoric stress tensor [8], or shear stress tensor [9]: τ (with components $\tau_{\alpha\beta}$)

The first two are rather straight-forward (but can be elaborated on a little bit more if you need it), but the third is a little more complicated. We generally regard the stress tensor as traceless

and symmetric (refer to Chapter 1). For a Newtonian fluid viscous stress is proportional to velocity gradients:

$$\boldsymbol{\tau} = \mu \left\{ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right\} + \lambda (\nabla \cdot \mathbf{u}) \mathbf{I} = 2\mu \mathcal{D}(\mathbf{u}) + \lambda (\nabla \cdot \mathbf{u}) \mathbf{I} \quad (4.60)$$

where $\mathcal{D}(\mathbf{u}) = \frac{1}{2} \left\{ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right\}$ is the deformation tensor, and $\lambda \approx -\frac{2}{3}\mu$. Note that in incompressible flow, the viscous stress tensor in Eq. (4.60) is a bit more easy with the $\lambda(\nabla \cdot \mathbf{u})$ term equal to zero.

In index notation, the viscous stress can be expressed as

$$\tau_{\alpha\beta} = \mu \left(\frac{\partial u_\alpha}{\partial \beta} + \frac{\partial u_\beta}{\partial \alpha} \right) + \delta_{\alpha\beta} \lambda \frac{\partial u_\gamma}{\partial \gamma} \quad (4.61)$$

That is, the deviatoric of the deformation rate tensor is identified to the deviatoric of the stress tensor, up to a factor μ . From [8] $\delta_{\alpha\beta}$ is the Kronecker delta. μ and λ are proportionality constants associated with the assumption that stress depends on strain linearly; μ is called the first coefficient of viscosity or shear viscosity (usually just called “viscosity”) and λ is the second coefficient of viscosity or volume viscosity (and it is related to bulk viscosity). The value of λ , which produces a viscous effect associated with volume change, is very difficult to determine, not even its sign is known with absolute certainty. Even in compressible flows, the term involving λ is often negligible; however it can occasionally be important even in nearly incompressible flows and is a matter of controversy. When taken nonzero, the most common approximation is $\lambda \approx -\frac{2}{3}\mu$. **In this case, for compressible flow, the viscous stress tensor is symmetric and traceless.**

Refer to Chapter 1, if we absorb the pressure term $p\delta_{\alpha\beta}$ and the viscous stress tensor $\tau_{\alpha\beta}$ into the single quantity: stress tensor $\sigma_{\alpha\beta} = -p\delta_{\alpha\beta} + \tau_{\alpha\beta} = -\left(p + \frac{2}{3}\mu \nabla \cdot \mathbf{u}\right)\delta_{\alpha\beta} + \mu(\partial_\beta u_\alpha + \partial_\alpha u_\beta)$, then the non-conservation form momentum equation in Eq. (4.58) becomes

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = \rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\tau} = \nabla \cdot \boldsymbol{\sigma} \quad (4.62)$$

or in index notation:

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha p + \partial_\beta \tau_{\alpha\beta} \quad (4.63)$$

Thus the momentum flux tensor \mathbf{P} in Eq. (4.58) can be extracted as:

$$\boxed{\mathbf{P} = p\mathbf{I} + \rho \mathbf{u} \otimes \mathbf{u} - \boldsymbol{\tau} = \rho \mathbf{u} \otimes \mathbf{u} - \boldsymbol{\sigma}} \quad (4.64)$$

in which $\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\tau}$ is the stress tensor. Or in index notation:

$$\boxed{P_{\alpha\beta} = p\delta_{\alpha\beta} + \rho u_\alpha u_\beta - \tau_{\alpha\beta} = \rho u_\alpha u_\beta - \sigma_{\alpha\beta}} \quad (4.65)$$

in which $\sigma_{\alpha\beta} = -p\delta_{\alpha\beta} + \tau_{\alpha\beta}$ is the stress tensor.

4.3.2.2 The Momentum Flux Tensor in LB

The momentum flux tensor \mathbf{M} expressed in Eq. (4.53) relates to the second-order moments $\boldsymbol{\Pi}$ of the distribution functions. The components of $\boldsymbol{\Pi}$ can be calculated as follows [2, 10, 11]:

$$\begin{cases} \Pi^{\text{eq}} = \sum_i \mathbf{c}_i \mathbf{c}_i f_i^{\text{eq}} = c_s^2 \rho \mathbf{I} + \rho \mathbf{u} \otimes \mathbf{u} = p \mathbf{I} + \rho \mathbf{u} \otimes \mathbf{u} \\ \Pi^{\text{neq}} = \sum_i \mathbf{c}_i \mathbf{c}_i f_i^{\text{neq}} = -\frac{c_s^2 \tau \delta_t}{\nu} \boldsymbol{\tau} = -2c_s^2 \rho \tau \delta_t \mathbf{s} \end{cases} \quad (4.66)$$

or in index notation:

$$\begin{cases} \Pi_{\alpha\beta}^{\text{eq}} = \sum_i c_{i\alpha} c_{i\beta} f_i^{\text{eq}} = c_s^2 \rho \delta_{\alpha\beta} + \rho u_\alpha u_\beta = p \delta_{\alpha\beta} + \rho u_\alpha u_\beta \\ \Pi_{\alpha\beta}^{\text{neq}} = \sum_i c_{i\alpha} c_{i\beta} f_i^{\text{neq}} = -\frac{c_s^2 \tau \delta_t}{\nu} \tau_{\alpha\beta} = -2c_s^2 \rho \tau \delta_t s_{\alpha\beta} \end{cases} \quad (4.67)$$

In which, $\mathbf{s} = \mathcal{D}(\mathbf{u}) = \frac{1}{2} \{ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \}$ is the rate of strain tensor, with index notation $s_{\alpha\beta} = \frac{1}{2}(\partial_\beta u_\alpha + \partial_\alpha u_\beta)$. The viscous stress tensor $\boldsymbol{\tau} = \mu \{ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \} + \lambda (\nabla \cdot \mathbf{u}) \mathbf{I}$ in incompressible or weak compressible flow with component $\tau_{\alpha\beta} = \mu(\partial_\beta u_\alpha + \partial_\alpha u_\beta)$. Also, $\mu = \rho \nu$ is the dynamic viscosity with ν the kinematic viscosity. For Newtonian fluids, the rate of strain tensor \mathbf{s} and the viscous stress tensor $\boldsymbol{\tau}$ are related through $2\rho\nu\mathbf{s} = \boldsymbol{\tau}$.

We can expand the rate of strain tensor \mathbf{s} as

$$\mathbf{s} = \begin{bmatrix} s_{xx} & s_{xy} & s_{xz} \\ s_{yx} & s_{yy} & s_{yz} \\ s_{zx} & s_{zy} & s_{zz} \end{bmatrix} = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & \frac{1}{2} \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \\ \frac{1}{2} \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) & \frac{\partial v}{\partial y} & \frac{1}{2} \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \\ \frac{1}{2} \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) & \frac{1}{2} \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right) & \frac{\partial w}{\partial z} \end{bmatrix} \quad (4.68)$$

For **incompressible fluid**, both the rate of strain tensor \mathbf{s} and the viscous stress tensor $\boldsymbol{\tau}$ are symmetric and traceless. As discussed, for **compressible fluid**, the viscous stress tensor $\boldsymbol{\tau}$ is still symmetric and traceless, but the rate of strain tensor defined as $\mathbf{s} = \frac{1}{2} \{ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \}$ is symmetric but not traceless anymore.

First, we can see that the strain rate tensor can be calculated using local LB method if we can obtain $\Pi_{\alpha\beta}^{\text{neq}}$ from $\sum_i c_{i\alpha} c_{i\beta} f_i^{\text{neq}}$, by

$$s_{\alpha\beta} = -\frac{1}{2c_s^2 \tau \delta_t \rho} \Pi_{\alpha\beta}^{\text{neq}} \quad (4.69)$$

Thus, combine with Eq. (4.66), the momentum flux tensor from Eq. (4.52) become:

$$\begin{aligned} \mathbf{M} &= \Pi^{\text{eq}} + \left(1 - \frac{1}{2\tau} \right) \Pi^{\text{neq}} \\ &= (p \mathbf{I} + \rho \mathbf{u} \otimes \mathbf{u}) + \left(1 - \frac{1}{2\tau} \right) \left(-\frac{c_s^2 \tau \delta_t}{\nu} \right) \boldsymbol{\tau} \end{aligned} \quad (4.70)$$

And in index notation, combine with Eq. (4.67), the momentum flux tensor from Eq. (4.53) become:

$$\begin{aligned}
M_{\alpha\beta} &= \Pi_{\alpha\beta}^{\text{eq}} + \left(1 - \frac{1}{2\tau}\right) \Pi_{\alpha\beta}^{\text{neq}} \\
&= (p\delta_{\alpha\beta} + \rho u_\alpha u_\beta) + \left(1 - \frac{1}{2\tau}\right) \left(-\frac{c_s^2 \tau \delta_t}{\nu}\right) \tau_{\alpha\beta}
\end{aligned} \tag{4.71}$$

The mesoscopic flux \mathbf{M} in Eq. (4.70) should equal to the macroscopic flux $\mathbf{P} = p\mathbf{I} + \rho\mathbf{u} \otimes \mathbf{u} - \boldsymbol{\tau}$ in Eq. (4.64), or in index notation, The mesoscopic flux $M_{\alpha\beta}$ in Eq. (4.71) should equal to the macroscopic flux $P_{\alpha\beta} = p\delta_{\alpha\beta} + \rho u_\alpha u_\beta - \tau_{\alpha\beta}$ in Eq. (4.65). So we have

$$\left(1 - \frac{1}{2\tau}\right) \left(-\frac{c_s^2 \tau \delta_t}{\nu}\right) = -1 \tag{4.72}$$

Then we can derive the relationship between the relaxation time τ and the lattice kinematic viscosity ν as follows

$$\begin{cases} \tau = \frac{\nu}{c_s^2 \delta_t} + \frac{1}{2} = 3\nu + \frac{1}{2} \\ \nu = \left(\tau - \frac{1}{2}\right) c_s^2 \delta_t = \frac{\tau - 1/2}{3} \end{cases} \tag{4.73}$$

with $c_s^2 = \frac{1}{3}$, refer to Section 2.2. Please do not mess the relaxation time τ with the viscous stress tensor $\boldsymbol{\tau}$.

Additionally, refer Eq. (4.71) and Eq. (4.67), the viscous stress tensor can be calculated from f_i as

$$\tau_{\alpha\beta} = -\left(1 - \frac{1}{2\tau}\right) \sum_i c_{i\alpha} c_{i\beta} f_i^{\text{neq}} = -\frac{\nu}{c_s^2 \tau \delta_t} \sum_i c_{i\alpha} c_{i\beta} f_i^{\text{neq}} \tag{4.74}$$

where the non-equilibrium distribution is the deviation of f_i from equilibrium, as shown in Eq. (4.40). However, computing the stress tensor explicitly in this way is usually not a necessary step when performing simulations.

Up to now, we can update the momentum conservation equation as:

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla \cdot \mathbf{M} = 0 \quad \Rightarrow \quad \frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla \cdot (\rho\mathbf{u} \otimes \mathbf{u}) = -\nabla \cdot (p\mathbf{I}) + \nabla \cdot \boldsymbol{\tau} \tag{4.75}$$

Or in index notation, we can update the momentum conservation equation as:

$$\partial_t(\rho u_\alpha) + \partial_\beta M_{\alpha\beta} = 0 \quad \Rightarrow \quad \partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\beta(p\delta_{\alpha\beta}) + \partial_\beta \tau_{\alpha\beta} \tag{4.76}$$

Note that $\nabla \cdot (p\mathbf{I}) = \nabla p$ in Eq. (4.75) or $\partial_\beta(p\delta_{\alpha\beta}) = \partial_\alpha p$ in Eq. (4.76). We can see that the mesoscopic momentum conservation in Eq. (4.75) and Eq. (4.76) is equivalent to the macroscopic momentum conservation in Eq. (4.62) and Eq. (4.63)

Thus we can derive the macroscopic mass momentum conservation equations from the mesoscopic mass momentum conservation equations in Eq. (4.56) and Eq. (4.57) to recover the incompressible Navier-Stokes equations¹:

¹Need further discussion here.

$$\begin{cases} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \\ \frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \left\{ \mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right\} \end{cases} \quad (4.77)$$

or in index notation:

$$\begin{cases} \partial_t \rho + \partial_\alpha (\rho u_\alpha) = 0 \\ \partial_t (\rho u_\alpha) + \partial_\beta (\rho u_\alpha u_\beta) = -\partial_\alpha p + \partial_\beta \{ \mu (\partial_\beta u_\alpha + \partial_\alpha u_\beta) \} \end{cases} \quad (4.78)$$

In small Mach number limit, the density variation can be negligible. Thus one can further obtain the weak compressible Navier-Stokes equations shown in Eq. (1.41) [11], with index notation shown in Eq. (1.42).

4.3.2.3 Non-Equilibrium Second-Order Moment

This section will derive the relationship between the non-equilibrium part $\Pi_{\alpha\beta}^{\text{neq}}$ of the second-order moment $\Pi_{\alpha\beta}$ shown in Eq. (4.66) and macroscopic quantities. The results for the equilibrium part $\Pi_{\alpha\beta}^{\text{eq}} = \Gamma_{\alpha\beta}^{\text{eq}}$ of the second-order moment shown in Eq. (4.66) and Eq. (2.49) will be discussed in a separate section².

For the isothermal equation of state and the equilibrium distribution f_i^{eq} expanded only to $\mathcal{O}(\mathbf{u}^2)$, the derivation process will yield the following relation.

$$\Pi_{\alpha\beta}^{\text{neq}} = -c_s^2 \rho \tau \delta_t (\partial_\beta u_\alpha + \partial_\alpha u_\beta) = -2c_s^2 \rho \tau \delta_t s_{\alpha\beta} \quad (4.79)$$

in which, $s_{\alpha\beta} = \frac{1}{2}(\partial_\beta u_\alpha + \partial_\alpha u_\beta)$ is the rate of strain tensor.

First, we get the second order moment (i.e. multiplying by $c_{i\beta}c_{i\gamma}$ and then summing over i) of $\mathcal{O}(\epsilon^1)$ from Eq. (4.22). As discussed earlier, when using Eq. (4.22), to form second order moment, it's better to roll up the index α in $c_{i\alpha}\partial_\alpha^{(1)}$ term to γ with $c_{i\gamma}\partial_\gamma^{(1)}$ term in order to reserve the lowest index α to the time derivative $\partial_t^{(1)}$, $\partial_t^{(2)}$ and finally ∂_t term. Since the 3rd order tensor will be involved, we will use the tensor expression in this derivation process. Thus we have

$$\begin{aligned} & \partial_t^{(1)} \sum_i c_{i\alpha} c_{i\beta} f_i^{(0)} + \partial_\gamma^{(1)} \left(\sum_i c_{i\alpha} c_{i\beta} c_{i\gamma} f_i^{(0)} \right) + \frac{1}{\tau \delta_t} \sum_i c_{i\alpha} c_{i\beta} f_i^{(1)} \\ &= \left[\partial_t^{(1)} \Pi_{\alpha\beta}^{(0)} + \partial_\gamma^{(1)} \Pi_{\alpha\beta\gamma}^{(0)} + \frac{1}{\tau \delta_t} \Pi_{\alpha\beta}^{(1)} \right] = 0 \end{aligned} \quad (4.80)$$

Refer to Eq. (2.49), $\Pi_{\alpha\beta}^{(0)} = \Pi_{\alpha\beta}^{\text{eq}} = c_s^2 \rho \delta_{\alpha\beta} + \rho u_\alpha u_\beta$. Also, as introduced in [2, 12], the third order tensor:

$$\Pi_{\alpha\beta\gamma}^{(0)} = c_s^2 \rho (u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta}) + \rho u_\alpha u_\beta u_\gamma \quad (4.81)$$

Note that from Eq. (2.49), $\Pi_{\alpha\beta\gamma}^{(0)} \approx \Gamma_{\alpha\beta\gamma}^{\text{eq}} = c_s^2 \rho (u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta})$. The tensor $\Pi_{\alpha\beta\gamma}^{(0)}$ contained the term $(\rho u_\alpha u_\beta u_\gamma)$ from the exact kinetic theory. The reason why this term is missing in $\Gamma_{\alpha\beta\gamma}^{\text{eq}}$ is that we have truncated the equilibrium distribution f_i^{eq} expanded only to $\mathcal{O}(\mathbf{u}^2)$.

²This should be discussed in another chapter.

We also need to make use of a corollary of the product rule [13]; if ∂_* is a generic derivative and a , b , and c are generic variables, then

$$\begin{aligned}\partial_*(abc) &= a\partial_*(bc) + bc\partial_*(a) \\ &= a\partial_*(bc) + bc\partial_*(a) + ab\partial_*(c) - ab\partial_*(c) \\ &= a\partial_*(bc) + b\partial_*(ac) - ab\partial_*(c)\end{aligned}\tag{4.82}$$

We will now resolve the two equilibrium moment derivatives in separately, starting with the one which is the simplest to resolve:

$$\begin{aligned}\partial_\gamma^{(1)}\Pi_{\alpha\beta\gamma}^{(0)} &= \partial_\gamma^{(1)}\{c_s^2\rho(u_\alpha\delta_{\beta\gamma} + u_\beta\delta_{\alpha\gamma} + u_\gamma\delta_{\alpha\beta}) + \rho u_\alpha u_\beta u_\gamma\} \\ &= c_s^2\left\{\partial_\beta^{(1)}(\rho u_\alpha) + \partial_\alpha^{(1)}(\rho u_\beta)\right\} + c_s^2\delta_{\alpha\beta}\partial_\gamma^{(1)}(\rho u_\gamma) + \partial_\gamma^{(1)}(\rho u_\alpha u_\beta u_\gamma) \\ &= \boxed{c_s^2\left\{\rho\partial_\beta^{(1)}u_\alpha + u_\alpha\partial_\beta^{(1)}\rho + \rho\partial_\alpha^{(1)}u_\beta + u_\beta\partial_\alpha^{(1)}\rho\right\} + c_s^2\delta_{\alpha\beta}\partial_\gamma^{(1)}(\rho u_\gamma) + \partial_\gamma^{(1)}(\rho u_\alpha u_\beta u_\gamma)}\end{aligned}\tag{4.83}$$

The other equilibrium moment derivative is more complicated, and we will resolve it in steps. First of all, we apply the product rule in Eq. (4.82) and find

$$\begin{aligned}\partial_t^{(1)}\Pi_{\alpha\beta}^{(0)} &= \partial_t^{(1)}(c_s^2\rho\delta_{\alpha\beta} + \rho u_\alpha u_\beta) \\ &= \boxed{c_s^2\delta_{\alpha\beta}\partial_t^{(1)}\rho + u_\alpha\partial_t^{(1)}(\rho u_\beta) + u_\beta\partial_t^{(1)}(\rho u_\alpha) - u_\alpha u_\beta\partial_t^{(1)}\rho}\end{aligned}\tag{4.84}$$

We go back and get the zeroth order moment (i.e. multiplying by 1 and then summing over i , note that we roll up the index α in $c_{i\alpha}\partial_\alpha^{(1)}$ term to γ with $c_{i\gamma}\partial_\gamma^{(1)}$ term) of $\mathcal{O}(\epsilon^1)$ from Eq. (4.22), we get:

$$\mathcal{O}(\epsilon^1) : \quad \partial_t^{(1)}\sum_i f_i^{(0)} + \partial_\gamma^{(1)}\left(\sum_i c_{i\gamma}f_i^{(0)}\right) = 0\tag{4.85}$$

According to the mesoscopic conservation rules in Section 4.3.1.2, we get:

$$\boxed{\partial_t^{(1)}\rho = -\partial_\gamma^{(1)}(\rho u_\gamma)}\tag{4.86}$$

Thereafter we get the first order moment (i.e. multiplying by $c_{i\alpha}$ and then summing over i) of $\mathcal{O}(\epsilon^1)$ from Eq. (4.22), we get:

$$\mathcal{O}(\epsilon^1) : \quad \partial_t^{(1)}\sum_i c_{i\alpha}f_i^{(0)} + \partial_\gamma^{(1)}\left(\sum_i c_{i\alpha}c_{i\gamma}f_i^{(0)}\right) = \partial_t^{(1)}(\rho u_\alpha) + \partial_\gamma^{(1)}\Pi_{\alpha\gamma}^{(0)} = 0\tag{4.87}$$

Combine with the result of the equilibrium part of the second-order moments shown in Eq. (4.67), we derive the following equivalent forms:

$$\boxed{\partial_t^{(1)}(\rho u_\alpha) = -\partial_\gamma^{(1)}\Pi_{\alpha\gamma}^{(0)} = -\partial_\gamma^{(1)}(c_s^2\rho\delta_{\alpha\gamma} + \rho u_\alpha u_\gamma)}\tag{4.88a}$$

$$\boxed{\partial_t^{(1)}(\rho u_\beta) = -\partial_\gamma^{(1)}\Pi_{\beta\gamma}^{(0)} = -\partial_\gamma^{(1)}(c_s^2\rho\delta_{\beta\gamma} + \rho u_\beta u_\gamma)}\tag{4.88b}$$

Then we replace the time derivatives and subsequently rearrange:

$$\begin{aligned}
\partial_t^{(1)} \Pi_{\alpha\beta}^{(0)} &= -u_\alpha \partial_\gamma^{(1)} (c_s^2 \rho \delta_{\beta\gamma} + \rho u_\beta u_\gamma) - u_\beta \partial_\gamma^{(1)} (c_s^2 \rho \delta_{\alpha\gamma} + \rho u_\alpha u_\gamma) \\
&\quad + u_\alpha u_\beta \partial_\gamma^{(1)} (\rho u_\gamma) - c_s^2 \delta_{\alpha\beta} \partial_\gamma^{(1)} (\rho u_\gamma) \\
&= -\left\{ u_\alpha \partial_\gamma^{(1)} (\rho u_\beta u_\gamma) + u_\beta \partial_\gamma^{(1)} (\rho u_\alpha u_\gamma) - u_\alpha u_\beta \partial_\gamma^{(1)} (\rho u_\gamma) \right\} \\
&\quad - c_s^2 \left(u_\alpha \partial_\beta^{(1)} \rho + u_\beta \partial_\alpha^{(1)} \rho \right) - c_s^2 \delta_{\alpha\beta} \partial_\gamma^{(1)} (\rho u_\gamma)
\end{aligned} \tag{4.89}$$

Finally, the bracketed terms can be simplified by using the product rule in Eq. (4.82) in reverse,

$$\partial_t^{(1)} \Pi_{\alpha\beta}^{(0)} = -\partial_\gamma^{(1)} (\rho u_\alpha u_\beta u_\gamma) - c_s^2 \left(u_\alpha \partial_\beta^{(1)} \rho + u_\beta \partial_\alpha^{(1)} \rho \right) - c_s^2 \delta_{\alpha\beta} \partial_\gamma^{(1)} (\rho u_\gamma) \tag{4.90}$$

Now that we have explicit forms of the two equilibrium moment derivative terms. After using the product rule and having some terms cancel, we end up with the explicit expression:

$$\begin{aligned}
\Pi_{\alpha\beta}^{(1)} &= -\tau \delta_t \left(\partial_t^{(1)} \Pi_{\alpha\beta}^{(0)} + \partial_\gamma^{(1)} \Pi_{\alpha\beta\gamma}^{(0)} \right) \\
&= \boxed{-c_s^2 \rho \tau \delta_t \left(\partial_\beta^{(1)} u_\alpha + \partial_\alpha^{(1)} u_\beta \right)}
\end{aligned} \tag{4.91}$$

Thus we can finally obtain that

$$\Pi_{\alpha\beta}^{\text{neq}} = \epsilon \Pi_{\alpha\beta}^{(1)} = -c_s^2 \rho \tau \delta_t \left(\epsilon \partial_\beta^{(1)} u_\alpha + \epsilon \partial_\alpha^{(1)} u_\beta \right) = -c_s^2 \rho \tau \delta_t (\partial_\beta u_\alpha + \partial_\alpha u_\beta) \tag{4.92}$$

4.4 Non-Equilibrium Distribution Function

It also worth a deep discussion about f_i^{neq} defined in Eq. (4.40). The second moment of the non-equilibrium distribution function f_i^{neq} can be used to calculate the non-equilibrium part $\Pi_{\alpha\beta}^{\text{neq}}$ of the second-order moment.

From the relation between the first-order distribution functions $f_i^{(1)}$ and the equilibrium distribution functions f_i^{eq} as described in Eq. (4.24), we have:

$$f_i^{\text{neq}} = \epsilon f_i^{(1)} = -\epsilon \tau \delta_t \left(\frac{\partial}{\partial t_1} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}_1} \right) f_i^{\text{eq}} = -\tau \delta_t \left(\frac{\partial}{\partial t} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}} \right) f_i^{\text{eq}} = -\tau \delta_t D_i f_i^{\text{eq}} \tag{4.93}$$

in which we adopted the first order multi-scale approximation of ∂_t and $\nabla_{\mathbf{r}}$ defined in Eq. (4.6), as $\partial_t = \epsilon \partial_{t_1}$ and $\nabla_{\mathbf{r}} = \epsilon \nabla_{\mathbf{r}_1}$, and also, $D_i = \partial_t + \mathbf{c}_i \cdot \nabla_{\mathbf{r}} = \partial_t + c_{i\alpha} \partial_\alpha$ like the material derivative. Here the Einstein's summation rule is used, i.e., two repeated index means taking the summation over this index. Note that the first order Taylor expansion for space and time reads,

$$f_i(\mathbf{r} + \mathbf{c}_i \delta_t, t + \delta_t) = f_i(\mathbf{r}, t) + \delta_t \left(\frac{\partial}{\partial t} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}} \right) f_i(\mathbf{r}, t) + \mathcal{O}(\delta_t^2) = f_i(\mathbf{r}, t) + \delta_t D_i f_i(\mathbf{r}, t) + \mathcal{O}(\delta_t^2)$$

4.4.1 Flux Solver Method

Now we introduce a **Flux Solver Method** to solve the calculate the non-equilibrium distribution functions [1, 14].

Using first-order Taylor series expansion for space and time:

$$f_i^{\text{eq}}(\mathbf{r} - \mathbf{c}_i \delta_t, t - \delta_t) = f_i^{\text{eq}}(\mathbf{r}, t) + \frac{\partial}{\partial t} \{f_i^{\text{eq}}(\mathbf{r}, t)(-\delta_t)\} + \frac{\partial}{\partial \mathbf{r}} \cdot \{f_i(\mathbf{r}, t)(-\mathbf{c}_i \delta_t)\} + \mathcal{O}(\delta_t^2) \quad (4.94)$$

Thus we derive that:

$$f_i^{\text{eq}}(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r} - \mathbf{c}_i \delta_t, t - \delta_t) = \delta_t \left(\frac{\partial}{\partial t} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}} \right) f_i^{\text{eq}}(\mathbf{r}, t) + \mathcal{O}(\delta_t^2) \quad (4.95)$$

From the relation between the non-equilibrium distribution functions f_i^{neq} and the equilibrium distribution functions f_i^{eq} as described in Eq. (4.93), we have:

$$f_i^{\text{neq}} = -\tau \delta_t \left(\frac{\partial}{\partial t} + \mathbf{c}_i \cdot \nabla_{\mathbf{r}} \right) f_i^{\text{eq}} = -\tau \{f_i^{\text{eq}}(\mathbf{r}, t) - f_i^{\text{eq}}(\mathbf{r} - \mathbf{c}_i \delta_t, t - \delta_t)\} + \mathcal{O}(\delta_t^2) \quad (4.96)$$

This equation means that once we have the equilibrium distribution functions at the target cell in current time step and its surrounding cells in previous time step, we can have the full information of distribution functions at the target cell in current time step.

4.4.2 Multi-Scale Analysis Method

Reference [4, 5, 15, 16] provided a simplified method to calculate the non-equilibrium part of the distribution functions directly. The detailed derivation of this method using multiscale analysis can be found in reference [6]. Basically, all references use the same calculation form.

To find f_i^{neq} explicitly through $f_i^{\text{neq}} = \epsilon f_i^{(1)}$ and $f_i^{(1)} = -\tau \delta_t \left(\partial_t^{(1)} + c_{i\alpha} \partial_{\alpha}^{(1)} \right) f_i^{\text{eq}}$ as shown in Eq. (4.93), we can apply the time and space derivatives directly to the equilibrium distribution in Eq. (2.43c). First, we consider the time derivative:

$$\begin{aligned} \partial_t^{(1)} f_i^{\text{eq}} &= \partial_t^{(1)} \left\{ w_i \rho \left(1 + \frac{1}{c_s^2} c_{i\alpha} u_{\alpha} + \frac{1}{2c_s^4} Q_{i\alpha\beta} u_{\alpha} u_{\beta} \right) \right\} \\ &= \boxed{w_i \left\{ \partial_t^{(1)} \rho + \frac{1}{c_s^2} c_{i\alpha} \partial_t^{(1)} (\rho u_{\alpha}) + \frac{1}{2c_s^4} Q_{i\alpha\beta} \partial_t^{(1)} (\rho u_{\alpha} u_{\beta}) \right\}} \end{aligned} \quad (4.97)$$

Again, $Q_{i\alpha\beta} = c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta}$.

From the in multi-scale analysis in Eq. (4.86) and Eq. (4.88):

$$\partial_t^{(1)} \rho = \underbrace{-\partial_{\alpha}^{(1)} (\rho u_{\alpha})}_{\text{for zeroth order moment only}} \quad (4.98a)$$

$$\partial_t^{(1)} (\rho u_{\alpha}) = \underbrace{-\partial_{\beta}^{(1)} (c_s^2 \rho \delta_{\alpha\beta} + \rho u_{\alpha} u_{\beta})}_{\text{for first order moment only}} \quad (4.98b)$$

$$\partial_t^{(1)} (\rho u_{\alpha}) = \underbrace{-\partial_{\gamma}^{(1)} (c_s^2 \rho \delta_{\alpha\gamma} + \rho u_{\alpha} u_{\gamma})}_{\text{for second order moment only}} \quad (4.98c)$$

$$\partial_t^{(1)} (\rho u_{\beta}) = \underbrace{-\partial_{\gamma}^{(1)} (c_s^2 \rho \delta_{\beta\gamma} + \rho u_{\beta} u_{\gamma})}_{\text{for second order moment only}} \quad (4.98d)$$

Note that the *first order moment only* $\partial_t^{(1)}(\rho u_\alpha)$ will be used to for the $\frac{1}{c_s^2} c_{i\alpha} \partial_t^{(1)}(\rho u_\alpha)$ term, and the *second order moment only* $\partial_t^{(1)}(\rho u_\alpha)$ will be used to for the $\frac{1}{2c_s^4} Q_{i\alpha\beta} \partial_t^{(1)}(\rho u_\alpha u_\beta)$ term in the above time derivative equation. This is because the notation in the equilibrium distribution function f_i^{eq} is automatically reduced already.

Also, apply the product rule in Eq. (4.82) and then the product rule in reverse, we find

$$\begin{aligned}
 \partial_t^{(1)}(\rho u_\alpha u_\beta) &= u_\alpha \partial_t^{(1)}(\rho u_\beta) + u_\beta \partial_t^{(1)}(\rho u_\alpha) - u_\alpha u_\beta \partial_t^{(1)} \rho \\
 &= u_\alpha \left\{ -\partial_\gamma^{(1)} (c_s^2 \rho \delta_{\beta\gamma} + \rho u_\beta u_\gamma) \right\} + u_\beta \left\{ -\partial_\gamma^{(1)} (c_s^2 \rho \delta_{\alpha\gamma} + \rho u_\alpha u_\gamma) \right\} + u_\alpha u_\beta \partial_\gamma^{(1)}(\rho u_\gamma) \\
 &= -\left\{ u_\alpha \partial_\gamma^{(1)}(\rho u_\beta u_\gamma) + u_\beta \partial_\gamma^{(1)}(\rho u_\alpha u_\gamma) - u_\alpha u_\beta \partial_\gamma^{(1)}(\rho u_\gamma) \right\} \\
 &\quad - c_s^2 \left\{ u_\alpha \partial_\gamma^{(1)}(\rho \delta_{\beta\gamma}) + u_\beta \partial_\gamma^{(1)}(\rho \delta_{\alpha\gamma}) \right\} \\
 &= -\partial_\gamma^{(1)}(\rho u_\alpha u_\beta u_\gamma) - c_s^2 \left(u_\alpha \partial_\beta^{(1)} \rho + u_\beta \partial_\alpha^{(1)} \rho \right)
 \end{aligned} \tag{4.99}$$

Thus, we can update the equation:

$$\begin{aligned}
 \partial_t^{(1)} f_i^{\text{eq}} &= -w_i \left\{ \partial_\alpha^{(1)}(\rho u_\alpha) + c_{i\alpha} \partial_\alpha^{(1)} \rho + \frac{c_{i\alpha}}{c_s^2} \partial_\beta^{(1)}(\rho u_\alpha u_\beta) \right. \\
 &\quad \left. + \frac{Q_{i\alpha\beta}}{2c_s^4} \partial_\gamma^{(1)}(\rho u_\alpha u_\beta u_\gamma) + \frac{Q_{i\alpha\beta}}{2c_s^2} \left(u_\alpha \partial_\beta^{(1)} \rho + u_\beta \partial_\alpha^{(1)} \rho \right) \right\}
 \end{aligned} \tag{4.100}$$

Since $Q_{i\alpha\beta} = c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta}$ is symmetric in α and β , $Q_{i\alpha\beta} A_{\alpha\beta} = Q_{i\alpha\beta} A_{\beta\alpha}$ for any tensor $A_{\alpha\beta}$ [2] (this tensor product can be written as the double dot product shown in Section 2.2.1, as $\mathbf{Q}_i : \mathbf{A}$, thus this assumption is obvious). Thus we can simplify the time derivative:

$$\begin{aligned}
 \partial_t^{(1)} f_i^{\text{eq}} &= -w_i \left\{ \partial_\alpha^{(1)}(\rho u_\alpha) + c_{i\alpha} \partial_\alpha^{(1)} \rho + \frac{c_{i\alpha}}{c_s^2} \partial_\beta^{(1)}(\rho u_\alpha u_\beta) \right. \\
 &\quad \left. + \frac{Q_{i\alpha\beta}}{2c_s^4} \partial_\gamma^{(1)}(\rho u_\alpha u_\beta u_\gamma) + \frac{Q_{i\alpha\beta}}{c_s^2} u_\alpha \partial_\beta^{(1)} \rho \right\}
 \end{aligned} \tag{4.101}$$

Now we consider the spatial derivative. Note that the time derivative $c_{i\alpha} \partial_\alpha^{(1)}$ will also roll up the notation. The α will roll up to β when α is occupied, such as in $c_{i\alpha} u_\alpha$ term, and will roll up to γ when α and β are occupied, such as in $Q_{i\alpha\beta} u_\alpha u_\beta$ term. Thus

$$\begin{aligned}
 c_{i\alpha} \partial_\alpha^{(1)} f_i^{\text{eq}} &= c_{i\alpha,\beta,\gamma} \partial_{\alpha,\beta,\gamma}^{(1)} \left\{ w_i \rho \left(1 + \frac{1}{c_s^2} c_{i\alpha} u_\alpha + \frac{1}{2c_s^4} Q_{i\alpha\beta} u_\alpha u_\beta \right) \right\} \\
 &= w_i \left\{ c_{i\alpha} \partial_\alpha^{(1)} \rho + \frac{1}{c_s^2} c_{i\alpha} c_{i\beta} \partial_\beta^{(1)}(\rho u_\alpha) + \frac{1}{2c_s^4} Q_{i\alpha\beta} c_{i\gamma} \partial_\gamma^{(1)}(\rho u_\alpha u_\beta) \right\}
 \end{aligned} \tag{4.102}$$

In the spatial derivative equation, since $Q_{i\alpha\beta} = c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta}$, thus $c_{i\alpha} c_{i\beta} = Q_{i\alpha\beta} + c_s^2 \delta_{\alpha\beta}$, thus

$$\begin{aligned}
c_{i\alpha}\partial_\alpha^{(1)}f_i^{\text{eq}} &= w_i \left\{ c_{i\alpha}\partial_\alpha^{(1)}\rho + \frac{Q_{i\alpha\beta}}{c_s^2}\partial_\beta^{(1)}(\rho u_\alpha) + \delta_{\alpha\beta}\partial_\beta^{(1)}(\rho u_\alpha) + \frac{1}{2c_s^4}Q_{i\alpha\beta}c_{i\gamma}\partial_\gamma^{(1)}(\rho u_\alpha u_\beta) \right\} \\
&= w_i \left\{ c_{i\alpha}\partial_\alpha^{(1)}\rho + \frac{Q_{i\alpha\beta}}{c_s^2}\partial_\beta^{(1)}(\rho u_\alpha) + \partial_\alpha^{(1)}(\rho u_\alpha) + \frac{Q_{i\alpha\beta}}{2c_s^4}c_{i\gamma}\partial_\gamma^{(1)}(\rho u_\alpha u_\beta) \right\} \\
&= \boxed{w_i \left\{ c_{i\alpha}\partial_\alpha^{(1)}\rho + \frac{Q_{i\alpha\beta}}{c_s^2}\rho\partial_\beta^{(1)}u_\alpha + \frac{Q_{i\alpha\beta}}{c_s^2}u_\alpha\partial_\beta^{(1)}\rho + \partial_\alpha^{(1)}(\rho u_\alpha) + \frac{Q_{i\alpha\beta}}{2c_s^4}c_{i\gamma}\partial_\gamma^{(1)}(\rho u_\alpha u_\beta) \right\}}
\end{aligned} \tag{4.103}$$

Therefore:

$$\begin{aligned}
f_i^{(1)} &= -\tau\delta_t \left(\partial_t^{(1)} + c_{i\alpha}\partial_\alpha^{(1)} \right) f_i^{\text{eq}} \\
&= -\frac{w_i\tau\delta_t}{c_s^2} \left\{ Q_{i\alpha\beta}\rho\partial_\beta^{(1)}u_\alpha - c_{i\alpha}\partial_\beta^{(1)}(\rho u_\alpha u_\beta) + \frac{Q_{i\alpha\beta}}{2c_s^2}c_{i\gamma}\partial_\gamma^{(1)}(\rho u_\alpha u_\beta) - \frac{Q_{i\alpha\beta}}{2c_s^2}\partial_\gamma^{(1)}(\rho u_\alpha u_\beta u_\gamma) \right\}
\end{aligned} \tag{4.104}$$

Finally, from $f_i^{\text{neq}} = \epsilon f_i^{(1)}$ and the multi-scale expressions for spatial derivative in Eq. (4.7), we have

$$f_i^{\text{neq}} = -\frac{w_i\tau\delta_t}{c_s^2} \left\{ Q_{i\alpha\beta}\rho\partial_\beta u_\alpha - c_{i\alpha}\partial_\beta(\rho u_\alpha u_\beta) + \frac{Q_{i\alpha\beta}}{2c_s^2}c_{i\gamma}\partial_\gamma(\rho u_\alpha u_\beta) - \frac{Q_{i\alpha\beta}}{2c_s^2}\partial_\gamma(\rho u_\alpha u_\beta u_\gamma) \right\} \tag{4.105}$$

As terms with nonlinear velocity components do not contribute to $\Pi_{\alpha\beta}^{\text{neq}}$, it is reasonable to approximate f_i^{neq} by its linear term only [16], thus

$$f_i^{\text{neq}} \approx -\frac{w_i\rho\tau\delta_t}{c_s^2} Q_{i\alpha\beta}\partial_\beta u_\alpha \tag{4.106}$$

From the non-equilibrium second order moment in Eq. (4.79) $\Pi_{\alpha\beta}^{\text{neq}} = -c_s^2\rho\tau\delta_t(\partial_\beta u_\alpha + \partial_\alpha u_\beta)$, and refer to the symmetric tensor product rule in Section 4.4.2, we have $Q_{i\alpha\beta}\partial_\beta u_\alpha = Q_{i\alpha\beta}\partial_\alpha u_\beta$, thus

$$f_i^{\text{neq}} \approx -\frac{w_i\rho\tau\delta_t}{2c_s^2} Q_{i\alpha\beta}(\partial_\beta u_\alpha + \partial_\alpha u_\beta) = \frac{w_i}{2c_s^4} Q_{i\alpha\beta}\Pi_{\alpha\beta}^{\text{neq}} = -\frac{w_i\rho\tau\delta_t}{c_s^2} Q_{i\alpha\beta}s_{\alpha\beta} \tag{4.107}$$

in which, $s_{\alpha\beta} = \frac{1}{2}(\partial_\beta u_\alpha + \partial_\alpha u_\beta)$ is the rate of strain tensor.

If written in matrix form, we have:

$$f_i^{\text{neq}} \approx -\frac{w_i\rho\tau\delta_t}{2c_s^2} \mathbf{Q}_i : \left\{ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right\} = \frac{w_i}{2c_s^4} \mathbf{Q}_i : \mathbf{\Pi}^{\text{neq}} = -\frac{w_i\rho\tau\delta_t}{c_s^2} \mathbf{Q}_i : \mathbf{s} \tag{4.108}$$

in which, $\mathbf{s} = \frac{1}{2} \left\{ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right\}$ is the rate of strain tensor.

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