

## Elements of the Lattice Boltzmann Method II: Kinetics and Hydrodynamics in One Dimension

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**Abstract.** Concepts of the lattice Boltzmann method are discussed in detail for the one-dimensional kinetic model. Various techniques of constructing lattice Boltzmann models are discussed, and novel collision integrals are derived. Geometry of the kinetic space and the role of the thermodynamic projector is elucidated.

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### 1 Introduction

In the first paper of this series [1], we have discussed some primary concepts of the lattice Boltzmann method for solving partial differential equations. The goal of the present paper is to extend the introduction of the lattice Boltzmann method to nonlinear problems while keeping the presentation as elementary as possible.

The outline of the paper is as follows. In Section 2 we consider the one-dimensional Navier-Stokes equations, and identify the requirements for lifting them to a kinetic equation. Construction of the kinetic equation begins in Section 3 where we derive the pertinent entropy function. In Section 4, we derive the corresponding equilibrium. In Section 5, we describe geometry of the phase space of kinetic equations, hydrodynamic and kinetic subspaces, and introduce the notion of detail balance as a geometrical statement. This section contains preliminary information which is used in the construction of collision integrals (Section 6). We develop general methods of constructing admissible collision integrals based on the entropy function. In Section 7, we consider linearization of

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collision integrals at equilibrium, and discuss in detail the notion of thermodynamic projector. In Section 8 we consider a special class of collision integrals which have the feature that their linearization is spectrally equivalent to the linearized Bhatnagar-Gross-Krook kinetic model (single relaxation time gradient models). In Section 9 we consider the entropic lattice Boltzmann scheme for these new models, and give a thorough analysis of the hydrodynamic limit of the discrete-time kinetic equation. We conclude in Section 10 with a brief discussion.

Finally, we did every effort to make the presentation self-containing, thus, references are kept at a minimal level. For a further reading on the lattice Boltzmann method, we direct the reader to the papers [2–5] and reviews [6–9]. Development of the entropic lattice Boltzmann method can be found in [10–20].

## 2 Hydrodynamic and kinetic equations

### 2.1 Navier-Stokes equations in one dimension

The target equations are the balance equations for the density  $\rho(x,t)$  and the momentum density  $j(x,t) = \rho u(x,t)$ :

$$\partial_t \rho + \partial_x(\rho u) = 0, \quad (2.1)$$

$$\partial_t(\rho u) + \partial_x P = 0, \quad (2.2)$$

$$P = \rho c_s^2 + \rho u^2 - 2\nu \rho \partial_x u. \quad (2.3)$$

This is the simplest example of the *Navier-Stokes equations*. We have written them in the ‘conservation laws + constitutive equation’ form. Now we have two equations for the conservation laws (for the density  $\rho$  and for the momentum  $j$ ). The constitutive equation for the pressure  $P$  (2.3) consists of two parts. The first part,  $P^E$ ,

$$P^E = \rho c_s^2 + \rho u^2, \quad (2.4)$$

is the value of the pressure at the equilibrium. If (2.4) is substituted instead of  $P$  in the balance equation for the momentum (2.2), the resulting non-dissipative hydrodynamic equations (2.1) and (2.2) form the simplest set of *Euler equations*. The second part of the pressure,  $P^{\text{neq}}$  is the non-equilibrium contribution,

$$P^{\text{NS}} = -2\nu \rho \partial_x u. \quad (2.5)$$

Parameter  $\nu > 0$  is the *viscosity coefficient*. While in the Eqs. (2.3) and (2.5) the viscosity coefficient appears simply as a parameter, we can infer that it will be expressed in terms of kinetic parameters of the kinetic models (relaxation time) once we will write it down (the same happened to the diffusion coefficient in the example of the advection-diffusion equation in [1]). The form of the constitutive relation (2.5) where the non-equilibrium pressure is proportional to the gradient of the momentum is typical of the *Newtonian fluid*.

## 2.2 Tailoring the moment system

The first step in setting up a kinetic system capable of reconstructing the target macroscopic equations (the one-dimensional Navier-Stokes equations in our example) is to find out how the moments of the populations should look like in the equilibrium. This is always possible even before one decides about the form of the equilibrium. To this end, we introduce the density  $\rho$ , the momentum flux  $j$ , and the pressure  $P$ :

$$\begin{aligned}\rho(f(x,t)) &= f_-(x,t) + f_0(x,t) + f_+(x,t), \\ j(f(x,t)) &= -cf_-(x,t) + cf_+(x,t), \\ P(f(x,t)) &= c^2f_-(x,t) + c^2f_+(x,t).\end{aligned}\tag{2.6}$$

Assuming the Bhatnagar-Gross-Krook (BGK) model [21]<sup>†</sup> for the populations  $f_i$ ,  $i = 1, \dots, n_d$ , where  $n_d = 3$  in our three-velocities example,  $i = 1$  corresponds to left-movers ( $c_1 = -c$ ),  $i = 2$  corresponds to stopped particles ( $c_2 = 0$ ), and  $i = 3$  corresponds to right-movers ( $c_3 = c$ ), the kinetic equation reads,

$$\partial_t f_i + c_i \partial_x f_i = -\frac{1}{\tau} (f_i - f_i^{\text{eq}}(\rho, j)).\tag{2.7}$$

Consistency requirement for the equilibrium population  $f_i^{\text{eq}}(\rho, j)$  assumes two local conservation laws (of the density and of the momentum),

$$\sum_{i=1}^{n_d} (f_i - f_i^{\text{eq}}(\rho, j)) = 0, \quad \sum_{i=1}^{n_d} c_i (f_i - f_i^{\text{eq}}(\rho, j)) = 0.\tag{2.8}$$

Eq. (2.7) is equivalently rewritten in terms of the three moments,

$$\begin{aligned}\partial_t \rho + \partial_x j &= 0, \\ \partial_t j + \partial_x P &= 0, \\ \partial_t P + \partial_x Q &= -\frac{1}{\tau} (P - P^{\text{eq}}).\end{aligned}\tag{2.9}$$

Here  $Q$  is the third-order moment (the *energy flux*),

$$Q = \sum_{i=1}^{n_d} f_i c_i^3.\tag{2.10}$$

Geometry of the three-velocities set  $c_i$  implies

$$Q = c^2 j, \text{ for any } f.\tag{2.11}$$

<sup>†</sup>One usually considers BGK for the analysis of the moment constraints for the sake of simplicity. However, the result of this analysis concerns only the equilibrium values of the non-conserved moments, and can be used for setting up different kinetic models on the same velocity sets as well. We shall consider other such models later in this paper.

Thus, the third-order moment is a linear combination of the locally conserved fields (it is proportional to the momentum flux), and the system (2.9) is closed.

When the relaxation time  $\tau$  is small, we expect that dynamics of the pressure  $P$  will be slaved by the dynamics of the locally conserved density and momentum, that is,  $P(x,t) = P(\rho(x,t), j(x,t))$ . In order to find out this dependence, we write down the invariance equation and solve it approximately to order  $\tau$  (see [1]). The invariance condition equates the time derivative of  $P(\rho, j)$  due to the dynamics of density and momentum to the time derivative of  $P$  due to the moment system (2.9):

$$\frac{\partial P}{\partial \rho} \partial_t \rho + \frac{\partial P}{\partial j} \partial_t j = \partial_t P. \tag{2.12}$$

Spelling out the time derivatives of the locally conserved fields, this gives

$$\frac{\partial P}{\partial \rho} (-\partial_x j) + \frac{\partial P}{\partial j} (-\partial_x P) = -\partial_x Q - \frac{1}{\tau} (P - P^{eq}). \tag{2.13}$$

This invariance equation is solved upon substituting

$$P = P^{(0)} + \tau P^{(1)} + \mathcal{O}(\tau^2), \tag{2.14}$$

where  $P^{(0)}$  annihilates the relaxation term, that is,  $P^{(0)} = P^{eq}$ , and we derive

$$P^{(1)} = \frac{\partial P^{eq}}{\partial \rho} (\partial_x j) + \frac{\partial P^{eq}}{\partial j} (\partial_x P^{eq}) - \partial_x Q^{eq}. \tag{2.15}$$

In order to evaluate the right hand side of this equation, we need an input for the equilibrium pressure. We require that the equilibrium pressure differs only by the terms of order  $\mathcal{O}(j^4)$  and higher from the Euler pressure (2.4), that is

$$P^{eq} = P^E + \mathcal{O}(j^4) = \rho c_s^2 + \frac{j^2}{\rho} + \mathcal{O}(j^4). \tag{2.16}$$

Moreover, the equilibrium value of the energy flux  $Q^{eq}$  is known due to the relation (2.11) which holds for any population, that is, also in the equilibrium  $Q^{eq} = c^2 j$ . With this input, we find

$$P^{(1)} = \underline{\rho(c_s^2 - c^2) \partial_x \left( \frac{j}{\rho} \right)} + (3c_s^2 - c^2) \left( \frac{j}{\rho} \right) \partial_x \rho + \partial_x \left( \frac{j^3}{\rho^2} \right) + \mathcal{O}(j^5). \tag{2.17}$$

The underlined term is the one which will reproduce the viscosity term in the target Navier-Stokes equation of our model. The rest of the terms are *anomalous*. Terms designated as  $\mathcal{O}(j^5)$  are due to any anomaly of the order  $\mathcal{O}(j^4)$  in (2.16).

The final step of the analysis is to find out what can be done in order to cancel as many as possible of the anomalies. Let us address what can be required in this kinetic model in order that it reconstructs the Navier-Stokes equations as closely as possible.

These requirements are imposed on the pressure tensor and other parameters such as the speed of sound, and they will be delegated in a form of constraints to the construction of the equilibrium. It is instructive to trace these requirements in orders of the momentum  $j$ . So, what can (and should) be required in this model?

- *Galilei invariance to order  $\mathcal{O}(j^4)$ .* It is absolutely crucial to require that the equilibrium pressure tensor should have the leading-order terms in the momentum as given by the Euler form:

$$P^{\text{eq}} = \rho c_s^2 + \frac{j^2}{\rho} + \mathcal{O}(j^4).$$

This we have already used when deriving (2.17). Anomalous terms of the order  $j^4$  can be tolerated since their effect is negligible once the Mach number is kept low. Some would prefer not to have any anomalous terms of whatever order in this expression. This is not critical, for two reasons: (i) Anomaly of the order  $\mathcal{O}(j^4)$  is separated from the  $j^2$  term by *two orders of magnitude*, and it is always easy to find operating window where the effect of the anomalous terms is *nihil*, and (ii) Even if the anomaly in the pressure tensor is cancelled, we still need to trade off the operating window because of the lower-order (cubic) anomalous terms in the energy flux (see below). Moreover, insisting on the cancellation of the anomaly in the pressure tensor is even counter-productive because, as we shall see it later in this paper, this inevitably leads to unstable schemes in the most challenging domain of low viscosities. *Therefore we shall not display anomalous terms of the order  $j^4$  and higher in any expression below unless it is required to avoid a confusion.*

- *Speed of sound leading to a cancellation of anomalous  $\mathcal{O}(j)$  terms in the non-equilibrium pressure.* If the speed of sound  $c_s$  in Eq. (2.17) is set as

$$3c_s^2 = c^2, \quad (2.18)$$

then the second term in this expression cancels, and we have

$$P^{(1)} = \underline{-2c_s^2 \rho \partial_x \left( \frac{j}{\rho} \right)} + \partial_x \left( \frac{j^3}{\rho^2} \right). \quad (2.19)$$

The two conditions, (2.16) and (2.18), are what we need to care about when constructing the equilibrium. Let us also answer the question: What *cannot* be required in this model?

- *Cubic anomaly in the non-equilibrium pressure.* After we managed to respect the two requirements on the equilibrium pressure and the speed of sound mentioned above, the non-equilibrium pressure becomes (2.19) which contains an anomalous term,  $\partial_x(j^3/\rho^2)$ . It comes due to the *anomalous cubic term in the energy flux*  $Q$ . This cubic anomaly cannot be eliminated by any choice of the equilibrium because of the lattice structure. Indeed,  $Q$  will always be the linear function of the momentum. If we

could have required

$$Q^{\text{MB}} = 3c_s^2 j + \frac{j^3}{\rho^2}, \quad (2.20)$$

then the cubic terms would cancel. This expression is well known in kinetic theory, and corresponds to the Maxwell-Boltzmann equilibrium distribution. However, in our three-velocity model the expression  $Q = c^2 j$  is *hard-wired* and cannot be negotiated. The only way to minimize this anomaly is to operate the model at low enough velocities. Experience shows that the maximal tolerable velocity  $u_{\text{max}}$  is of the order  $u_{\text{max}} \sim 0.1c_s$ .

Thus, assuming the equilibrium  $f^{\text{eq}}$  is found in such a way that the requirements (2.16) and (2.18) are verified, and the operating window is at sufficiently low Mach numbers, the kinetic model reconstructs the following Navier-Stokes equations at small  $\tau$ :

$$\partial_t \rho + \partial_x j = 0, \quad (2.21)$$

$$\partial_t j = -\partial_x \left( \rho c_s^2 + \frac{j^2}{\rho} \right) + 2(\tau c_s^2) \partial_x \left( \rho \partial_x \left( \frac{j}{\rho} \right) \right), \quad (2.22)$$

where the viscosity is identified as

$$\nu = \tau c_s^2. \quad (2.23)$$

These are the target Navier-Stokes equations. Now we proceed with finding the equilibrium populations.

### 3 Entropy function

The lesson we learned from the kinetic model for the advection equation [1] is that one should begin the construction with finding an appropriate entropy function  $H$ . In [1], this was relatively straightforward to do because for linear systems a general form of the entropy function is readily available. In the nonlinear case as here it is not immediately obvious what the entropy function should be, and so we begin with its derivation.

We define the equilibrium as the minimizer of a convex entropy function  $H$  under the constraints imposed by locally conserved fields,

$$H \rightarrow \min, \quad \sum_{i=1}^{n_d} f_i = \rho, \quad \sum_{i=1}^{n_d} c_i f_i = \rho u. \quad (3.1)$$

We shall look for the function  $H$  of the form,

$$H = h_0(f_0) + h_1(f_-) + h_1(f_+). \quad (3.2)$$

Convex functions of one variable  $h_0(z)$  and  $h_1(z)$  are yet unknown. The form (3.2) accounts for the symmetry between the left- and right-movers, that is, we have assumed

$h_-(z) = h_+(z) = h_1(z)$  (this assumption is certainly natural but it could be relaxed at the beginning of the construction, the result will nevertheless be the same as we obtain below).

Each individual member of the family of the convex functions (3.2), when used in the minimization problem (3.1), delivers a certain equilibrium. Equilibria for different  $H$  are not equivalent in their properties, so we need to find such pair of functions  $h_0$  and  $h_1$  which give us the 'right' equilibrium. The conditions deciding between the right and wrong equilibria were found in the previous section upon the analysis of the kinetic equation (2.7): The right equilibrium must deliver the pressure (2.16), whereas the speed of sound in this expression must satisfy (2.18). In this section we shall use the pair density-velocity  $(\rho, u)$  instead of density-momentum  $(\rho, j)$ , and the condition for the equilibrium pressure reads:

$$P^{\text{eq}} = \sum_{i=1}^{n_d} f_i^{\text{eq}} c_i c_i = \rho c_s^2 + \rho u^2. \tag{3.3}$$

It is important to digest the difference between the constraints in the minimization problem (3.1) and the constraint (3.3). The former are the definitions of the locally conserved fields (mass and momentum) whereas (3.3) is the *implication* of the equilibrium (and hence of the choice of the entropy function in (3.1)) for the non-conserved field  $P$  at equilibrium. In other words, (3.3) is the equilibrium piece of the constitutive relation (2.4), and cannot be treated on equal footing with the *definitions* of the locally conserved fields. Thus, it is absolutely meaningless to include (3.3) into the list of the constraints in (3.1), rather, it must be *verified* by the equilibrium found in (3.1).

In the next step, we formulate the requirement (3.3) as the implication of the solution of the minimization problem (3.1). Using the entropy function of the form (3.2), we introduce the derivatives  $dh_0(z)/dz$  and  $dh_1(z)/dz$ , and write the extremum condition in terms of Lagrange multipliers

$$\begin{aligned} \left. \frac{dh_0}{dz} \right|_{f_0^{\text{eq}}} &= \chi, \\ \left. \frac{dh_1}{dz} \right|_{f_-^{\text{eq}}} &= \chi - \lambda c, \\ \left. \frac{dh_1}{dz} \right|_{f_+^{\text{eq}}} &= \chi + \lambda c, \end{aligned} \tag{3.4}$$

where  $\chi$  and  $\lambda$  are the Lagrange multipliers corresponding to the density and the momentum constraints, respectively. Denoting  $\mu_0$  and  $\mu_1$  the inverse of the derivatives  $dh_{0,1}/dz$ ,

$$\mu_0(z) = \left[ \frac{dh_0}{dz} \right]^{-1}, \quad \mu_1(z) = \left[ \frac{dh_1}{dz} \right]^{-1},$$

we obtain

$$\begin{aligned} f_0^{\text{eq}} &= \mu_0(\chi), \\ f_-^{\text{eq}} &= \mu_1(\chi - \lambda c), \\ f_+^{\text{eq}} &= \mu_1(\chi + \lambda c), \end{aligned} \quad (3.5)$$

The Lagrange multipliers  $\chi$  and  $\lambda$  are (implicitly) related to  $\rho$  and  $\rho u$  upon substitution of the equilibria (3.5) into the constraints in (3.1). This gives

$$\begin{aligned} \mu_0(\chi) + \mu_1(\chi + \lambda c) + \mu_1(\chi - \lambda c) &= \rho, \\ c\mu_1(\chi + \lambda c) - c\mu_1(\chi - \lambda c) &= \rho u. \end{aligned} \quad (3.6)$$

The condition for the pressure at the equilibrium (3.3) then reads,

$$c^2\mu_1(\chi + \lambda c) + c^2\mu_1(\chi - \lambda c) - (\rho u^2 + \rho c_s^2) = 0. \quad (3.7)$$

For the time being, the speed of sound  $c_s$  in (3.7) will be considered as a free parameter (we shall see below that the choice of the speed of sound is a consistency condition). Expressing  $\rho$  and  $u$  in the right hand side of (3.7) in terms of (3.6) we rewrite the condition for the equilibrium pressure (3.7) in terms of the functions  $\mu_0$  and  $\mu_1$

$$\begin{aligned} c^2[\mu_1(\chi + \lambda c) + \mu_1(\chi - \lambda c)] - \frac{c^2[\mu_1(\chi + \lambda c) - \mu_1(\chi - \lambda c)]^2}{\mu_0(\chi) + \mu_1(\chi + \lambda c) + \mu_1(\chi - \lambda c)} \\ - c_s^2[\mu_0(\chi) + \mu_1(\chi + \lambda c) + \mu_1(\chi - \lambda c)] = 0. \end{aligned} \quad (3.8)$$

Eq. (3.8) is a nonlinear *functional* equation for the functions  $\mu_0$  and  $\mu_1$  (and hence for the functions  $h_0$  and  $h_1$  constituting the entropy), containing also the parameter  $c_s$ . The functional Eq. (3.8) is the central point in the construction of the entropy functions of the lattice Boltzmann method [11]. The entropy functions which satisfy (3.8) are called *perfect entropy functions*.

We shall now solve Eq. (3.8) approximately by using a Taylor series expansion to order  $\lambda^2$  around  $\lambda = 0$ . This solution will set the accuracy of the model to be applicable for simulations of low Mach number flows, that is, it will satisfy the pressure condition (that is, it will differ from (3.8) by terms of order  $u^4$  and higher, see previous section). We write,

$$\mu_1(\chi \pm \lambda c) = \mu_1(\chi) \pm \lambda c \frac{d\mu_1(\chi)}{d\chi} + \frac{1}{2}(\lambda c)^2 \frac{d^2\mu_1(\chi)}{d\chi^2} + \mathcal{O}(\lambda^3). \quad (3.9)$$

Substituting this expansion into Eq. (3.8), we require that the terms of the order  $\lambda^0$  and  $\lambda^2$  are equal to zero (terms of the order  $\lambda$  cancel out identically). After a few algebra one obtains a system of an ordinary differential and an algebraic equations:

$$\begin{aligned} \mu_0(\chi) &= 2 \left( \frac{c^2}{c_s^2} - 1 \right) \mu_1(\chi), \\ \left( \frac{d\mu_1(\chi)}{d\chi} \right) \left( \frac{d\mu_1(\chi)}{d\chi} \right) &= \frac{1}{2} \left( \frac{c^2}{c_s^2} - 1 \right) \mu_1(\chi) \frac{d^2\mu_1(\chi)}{d\chi^2}. \end{aligned} \quad (3.10)$$



The speed of sound  $c_s$  must now be chosen in such a way that the differential equation in the last line of (3.10) admits solutions compatible with the concavity requirement for the entropy function (3.2). At this point we turn our attention to the requirement on the speed of sound which we have already derived while analyzing the hydrodynamic limit, namely (2.18). If we set in (3.10):

$$c_s = \frac{1}{\sqrt{3}}c, \quad (3.11)$$

this results in the ordinary differential equation,

$$\left(\frac{d\mu_1(\chi)}{d\chi}\right)\left(\frac{d\mu_1(\chi)}{d\chi}\right) = \mu_1(\chi)\frac{d^2\mu_1(\chi)}{d\chi^2}. \quad (3.12)$$

The latter equation admits a special solution (see also Appendix A.1 for the general solution to this equation)

$$\mu_1(\chi) = e^{\chi-1}, \quad (3.13)$$

and from the algebraic equation in (3.10) it follows

$$\mu_0(\chi) = 4e^{\chi-1}. \quad (3.14)$$

The derivatives of the functions  $h_0$  and  $h_1$  are found upon inverting the functions  $\mu_0$  and  $\mu_1$ ,

$$\frac{dh_0}{d\chi} = \ln\left(\frac{\chi}{4}\right) + 1, \quad \frac{dh_1}{d\chi} = \ln\chi + 1, \quad (3.15)$$

whereupon

$$h_0 = \chi \ln\left(\frac{\chi}{4}\right), \quad h_1 = \chi \ln\chi. \quad (3.16)$$

Finally, using the latter functions in (3.2), we find the solution for the entropy function:

$$H = f_0 \ln\left(\frac{f_0}{4}\right) + f_- \ln f_- + f_+ \ln f_+. \quad (3.17)$$

By looking at the result (3.17), we recognize that this entropy function is of the Boltzmann type. Thus, it could be also derived from *Boltzmann's ansatz* (see Appendix A.2). Let us now verify that the equilibrium corresponding to the entropy function (3.17) indeed satisfies the condition for the equilibrium pressure (3.3) for small values of the velocity  $u$ . In order to do this, we need to evaluate the equilibrium populations as a function of  $u$ . Exact equilibrium can actually be found (see the next section, Eq. (4.1)). However, for the present purpose of verification, we do not even need the full solution, rather, just a few terms of its *expansion around the zero-velocity equilibrium*. Such approximation is easily obtained by expanding the Lagrange multipliers  $\chi$  and  $\lambda$  into a series in the powers of  $u$

(see Appendix A.3). The result of this expansion up to order  $u^2$  reads:

$$\begin{aligned} f_0^{\text{eq}} &= \frac{2\rho}{3} \left( 1 - \frac{u^2}{2c_s^2} \right) + \mathcal{O}(u^3) \\ f_-^{\text{eq}} &= \frac{\rho}{6} \left( 1 - \frac{uc}{c_s^2} + \frac{u^2}{c_s^2} \right) + \mathcal{O}(u^3) \\ f_+^{\text{eq}} &= \frac{\rho}{6} \left( 1 + \frac{uc}{c_s^2} + \frac{u^2}{c_s^2} \right) + \mathcal{O}(u^3). \end{aligned} \quad (3.18)$$

Here the speed of sound is not arbitrary anymore but is given by the expression (3.11). By retaining the terms spelled out explicitly in (3.18), we evaluate the equilibrium pressure,

$$\begin{aligned} P^{\text{eq}} &= \sum_{i=1}^{n_d} f_i^{\text{eq}} c_i^2 = c^2 f_-^{\text{eq}} + c^2 f_+^{\text{eq}} \\ &= \rho c_s^2 + \rho u^2 + \mathcal{O}(u^4). \end{aligned} \quad (3.19)$$

Note that the odd-order terms  $u^3$ , though they are not explicitly written in (3.18), do not contribute (cancel out) in the equilibrium pressure (3.19). Thus, the equilibrium corresponding to the entropy function (3.17) satisfy the equilibrium pressure condition (3.3) to the desired order of accuracy in the Mach number, so the desired perfect entropy function (3.17) is derived.

## 4 Equilibrium

Once the entropy function (3.17) is derived, we can ask for the equilibria which minimize  $H$  (3.17) subject to the fixed density  $\rho$  and momentum density  $\rho u$ . In the example considered here we find analytically the local equilibrium of the  $H$ -function (3.17),

$$\begin{aligned} f_0^{\text{eq}}(\rho, u) &= \frac{2\rho}{3} \left( 2 - \sqrt{1 + \text{Ma}^2} \right), \\ f_+^{\text{eq}}(\rho, u) &= \frac{\rho}{3} \left( \frac{uc - c_s^2}{2c_s^2} + \sqrt{1 + \text{Ma}^2} \right), \\ f_-^{\text{eq}}(\rho, u) &= \frac{\rho}{3} \left( -\frac{uc + c_s^2}{2c_s^2} + \sqrt{1 + \text{Ma}^2} \right), \end{aligned} \quad (4.1)$$

where  $\text{Ma}^2 = u^2/c_s^2$  is the Mach number squared,  $c_s = c/\sqrt{3}$ .

Derivation of the equilibrium populations (4.1) is straightforward. Denoting the exponentials of Lagrange multipliers corresponding to the momentum conservation as  $Y$ ,

$$Y = e^{c\lambda}, \quad Y^{-1} = e^{-c\lambda}, \quad (4.2)$$

we write the system of constraints as follows

$$\begin{aligned} e^\chi \left( 4 + Y + \frac{1}{Y} \right) &= \rho, \\ e^\chi c \left( Y - \frac{1}{Y} \right) &= \rho u. \end{aligned} \tag{4.3}$$

Dividing the second equation by the first, we derive a quadratic equation for  $Y$ :

$$\left( 1 - \frac{u}{c} \right) Y^2 - \frac{4u}{c} Y - \left( 1 + \frac{u}{c} \right) = 0. \tag{4.4}$$

The relevant root of this equation is the one which tends to 1 as  $u$  tends to 0. Taking into account the definition of the speed of sound for this model,  $c_s = c/\sqrt{3}$ , this root is written as

$$Y = \frac{\frac{2u}{\sqrt{3}c_s} + \sqrt{1 + \frac{u^2}{c_s^2}}}{1 - \frac{u}{\sqrt{3}c_s}}. \tag{4.5}$$

Substituting this solution into the density equation, we derive the function  $e^\chi$ , and, after some algebra, the equilibria in the form (4.1).

We have already encountered the equilibrium populations when discussing the kinetic model for the advection-diffusion equation in [1]: equilibrium functions were obtained from (4.1) by fixing the velocity  $u$  at a constant value  $v$ .

Let us find it out when the equilibria (4.1) have the meaning of populations, that is, when they are positive. We easily see that this is dictated by the sign of the populations of no-moving particles  $f_0^{\text{eq}}$ :

$$f_0^{\text{eq}}(\rho, u) > 0, \text{ when } |u| < c. \tag{4.6}$$

When  $|u|$  exceeds  $c$ , the populations of the moving particles stay positive but the population  $f_0^{\text{eq}}$  does not. That is, for  $|u| > c$ , there is no equilibrium, the problem of minimization of the entropy function (3.17) ceases to exist. Some telling values of the equilibria are collected in (4.7):

$f_i^{\text{eq}}$	$u = c$	$u = -c$	$u = 0$
$f_0^{\text{eq}}$	0	0	$\frac{2}{3}\rho$
$f_+^{\text{eq}}$	$\rho$	0	$\frac{1}{6}\rho$
$f_-^{\text{eq}}$	0	$\rho$	$\frac{1}{6}\rho$

(4.7)

The fact that the equilibria do not exist when the absolute value of the average velocity  $u$  exceeds the maximal speed  $c$  in the system is quite understandable, and is not a concern here. Indeed, by the construction, we are anyway restricted to small values of the Mach number  $\text{Ma} = |u|/c$ . More precisely, the order of the accuracy of the model as a tool to recover the Navier-Stokes equation is restricted by the terms of the order  $(u/c)^4$  in the

equilibrium pressure, and, moreover, by the terms of the order  $(u/c)^3$  in the equilibrium energy flux.

For the sake of completeness, we report the exact form of the equilibrium pressure corresponding to the equilibrium (4.1):

$$P^{\text{eq}} = \sum_{i=1}^{n_d} f_i^{\text{eq}} c_i^2 = \rho c_s^2 \left( 2\sqrt{1 + \frac{u^2}{c_s^2}} - 1 \right). \quad (4.8)$$

Expanding this expression to the order  $\text{Ma}^4$ , we obtain

$$P^{\text{eq}} = \rho c_s^2 \left( 1 + \text{Ma}^2 - \frac{1}{4} \text{Ma}^4 + \mathcal{O}(\text{Ma}^6) \right). \quad (4.9)$$

We see that, for small Mach numbers, this expression differs from the Eulerian pressure  $P^E = \rho c_s^2 (1 + \text{Ma}^2)$  only by a vanishing term  $\rho c_s^2 \text{Ma}^4 / 4$ , as already reported.

Our next step towards the lattice Boltzmann scheme is to write up a set of kinetic equations (continuous time and space),

$$\partial_t f_i + c_i \partial_x f_i = Q_i, \quad i = -, 0, +. \quad (4.10)$$

Since we have derived equilibrium populations explicitly, we can write the collision integral  $Q_i$  in (4.10) in the BGK form,

$$Q_i = -\frac{1}{\tau} (f_i - f_i^{\text{eq}}(\rho(f), u(f))), \quad (4.11)$$

and thus the BGK kinetic model (2.7) is set up completely.

However, it is more instructive to develop general methods for constructing collision integrals. Indeed, as we have seen it above, evaluation of the equilibrium required solving a set of algebraic equation like we did it in (4.4). We managed to solve the problem here (it was simple) but we cannot expect that explicit evaluation of  $f^{\text{eq}}$  is possible always (and actually it is not always possible). In the next section, we shall develop very general principles of constructing collision integrals for kinetic models.

## 5 Hydrodynamic and kinetic subspaces

Here it is most convenient to use vector notations. We remind that the populations are represented by three-dimensional ( $n_d = 3$ ) column-vectors  $f$  which we write using the natural coordinate system corresponding to the components  $f_i$ . The three-dimensional space of the column-vectors will be denoted as  $\mathcal{E}$ . The column-vectors with nonnegative components  $f_i \geq 0$  build a cone  $\mathcal{F} \subset \mathcal{E}$  (the phase space). Elements of the conjugated space will be denoted as row-vectors  $e^T$  where  $T$  stands for transposition,

$$e^T = ( e_1 \quad e_2 \quad e_3 ). \quad (5.1)$$

We consider the standard scalar product (or inner product, or dot-product in some literature) between the column-vectors and the row-vectors

$$e^T \cdot f = f^T \cdot e = (e_1 \ e_2 \ e_3) \begin{pmatrix} f_1 \\ f_2 \\ f_3 \end{pmatrix} = e_1 f_1 + e_2 f_2 + e_3 f_3. \quad (5.2)$$

In the three-dimensional linear space of row-vectors  $\mathcal{E}^T$ , let us introduce the two-dimensional linear subspace  $\mathcal{H}^T$  spanned by the two linearly independent row-vectors  $h_\rho^T$  and  $h_u^T$ , where

$$h_\rho^T = (1 \ 1 \ 1), \quad h_u^T = (-1 \ 0 \ 1). \quad (5.3)$$

Any row-vector  $h^T$  from the subspace  $\mathcal{H}^T$  can be represented as a linear combination of the row-vectors (5.3),

$$h^T \in \mathcal{H}^T, \quad \text{if and only if} \quad h^T = a_\rho h_\rho^T + a_u h_u^T. \quad (5.4)$$

The subspace  $\mathcal{H}^T$  is called the *hydrodynamic subspace* (of the space  $\mathcal{E}^T$ ) because the locally conserved (hydrodynamic) fields  $\rho$  and  $\rho u$  are expressed as the scalar products between the row-vectors (5.3) and the column-vectors of the populations,

$$\rho = h_\rho^T \cdot f, \quad \rho u = c h_u^T \cdot f. \quad (5.5)$$

A few comments are in order here. The row-vectors (5.3) form a basis, that is, a maximally linear independent system of the hydrodynamic subspace  $\mathcal{H}^T$ . They are indeed linearly independent (check this!) and even orthogonal to each other: if we make the column-vector  $h_u$  by transposing the row-vector  $h_u^T$ , then

$$h_\rho^T \cdot h_u = 0.$$

This is convenient but not really necessary, any other choice of the basis to represent  $\mathcal{H}^T$  would also do. The only important thing is the dimension, the number of the basis vectors must be equal to the number of the linearly independent conservation laws (in our case it is two).

Now let us consider the subspace  $\mathcal{H} \subset \mathcal{E}$  which consists of the column-vectors obtained by the transposition of the row-vectors  $h^T \in \mathcal{H}^T$ ,

$$\mathcal{H} = (\mathcal{H}^T)^T. \quad (5.6)$$

The *kinetic subspace*  $\mathcal{K}^T \subset \mathcal{E}^T$  consists of all row-vectors  $k^T$  which are orthogonal to the subspace  $\mathcal{H}$

$$k^T \in \mathcal{K}^T \quad \text{if and only if} \quad k^T \cdot h \quad \text{for any} \quad h \in \mathcal{H}. \quad (5.7)$$

This is the general definition valid for any construction of the minimal kinetic model. In our case the space  $\mathcal{E}^T$  is three-dimensional and the hydrodynamic subspace  $\mathcal{H}^T$  is two-dimensional (three populations and two locally conserved fields, respectively), so the

kinetic subspace is one-dimensional. It is convenient to represent the kinetic subspace as a line spanned by the row-vector  $g^T$ ,

$$g^T = ( 1 \quad -2 \quad 1 ). \tag{5.8}$$

It is straightforward to verify that the row-vector  $g^T$  (5.8) is orthogonal to any of the column-vectors of the transposed hydrodynamic subspace  $\mathcal{H}$ , that is,

$$g^T \perp \mathcal{H}.$$

Indeed, any column-vector  $h \in \mathcal{H}$  has the form  $h = ah_\rho + bh_u$ , where  $a$  and  $b$  are constants. Therefore, by linearity, it is sufficient to prove that  $g^T \cdot h_\rho = 0$  and  $g^T \cdot h_u = 0$ . The latter is obvious.

Thus, all row-vectors of the kinetic subspace are represented as

$$k^T = ag^T = ( a \quad -2a \quad a ), \quad -\infty < a < \infty. \tag{5.9}$$

In a sequel we shall also need a special representation of the kinetic row-vector  $g^T$  as a difference of two row-vectors with non-negative components:

$$\begin{aligned} g^T &= g^{T+} - g^{T-}, \\ g^{T+} &= ( 1 \quad 0 \quad 1 ), \\ g^{T-} &= ( 0 \quad 2 \quad 0 ). \end{aligned} \tag{5.10}$$

This is called a *stoichiometric representation*, and we shall later explain why this has to do with the established notion of chemical kinetics.

The choice of the basis row-vector  $g^T$  (5.8) to build the kinetic subspace  $\mathcal{K}^T$  is not unique (we could take any row-vector  $ag^T$  instead). In practice, it is usually convenient to choose the basis of the kinetic subspace in such a way that as many as possible of their components are integer (this saves computational time in the numerical realization). This was our motivation when choosing  $g^T$  (5.8).

Summarizing, we have decomposed the space of row-vectors into two subspaces, the hydrodynamic and the kinetic subspace,

$$\mathcal{E}^T = \mathcal{H}^T + \mathcal{K}^T. \tag{5.11}$$

Such a decomposition is unique and is *required* as the first step in the construction of any kinetic model. The hydrodynamic subspace supports all the local conservations (density and momentum in our case), while 'all the rest of  $\mathcal{E}^T$ ' is non-conserved and thus belongs to the kinetic subspace. The decomposition (5.11) is always a 'doable' exercise for any set of discrete velocities and a given set of local conservation laws.

We conclude this section with a simple but very useful consequence of the decomposition (5.11), namely, a different specification of the equilibrium states. To that end, we

need to introduce the column-vector of the partial derivatives of the entropy function  $H$  (3.17),

$$\nabla H = \begin{pmatrix} (\partial H / \partial f_1) \\ (\partial H / \partial f_2) \\ (\partial H / \partial f_3) \end{pmatrix} = \begin{pmatrix} \ln(f_-) + 1 \\ \ln(f_0/4) + 1 \\ \ln(f_-) + 1 \end{pmatrix}. \tag{5.12}$$

Equilibrium states furnish the minimum of  $H$  under fixed locally conserved fields. Thus,  $\nabla H$  at the equilibrium is a linear combination of the gradients of the constraints,

$$\nabla H|_{f^{eq}} = \chi h_\rho + \lambda h_u, \tag{5.13}$$

or, which is the same,  $\nabla H$  at equilibrium belongs to the transposition of the hydrodynamic subspace,

$$\nabla H|_{f^{eq}} \in \mathcal{H}. \tag{5.14}$$

Now, the kinetic subspace was defined as the orthogonal to  $\mathcal{H}$ , therefore, the equilibria are also *defined* as those states at which the column-vector  $\nabla H$  becomes orthogonal to the kinetic subspace of row-vectors,

$$\nabla H|_{f^{eq}} \perp \mathcal{K}^T. \tag{5.15}$$

The latter statement can be written in the form of an equation,

$$g^T \cdot \nabla H|_{f^{eq}} = 0. \tag{5.16}$$

Together with the constraints,  $h_\rho^T \cdot f^{eq} = \rho$ ,  $ch_u^T \cdot f^{eq} = \rho u$ , Eq. (5.16) forms a set of three equations for three components of the equilibrium row-vector  $f^{eq}$ . The equilibrium condition in this form is called *detailed balance*.

Let us to prove with a direct computation that this system of equations again leads to the equilibrium (4.1). Computing the scalar product of the row-vector  $g^T$  (5.8) with the column-vector  $\nabla H$  (5.12), we write the detailed balance (5.16) explicitly,

$$16f_+^{eq} f_-^{eq} = (f_0^{eq})^2. \tag{5.17}$$

With the definition of the hydrodynamic fields at the equilibrium,

$$f_-^{eq} + f_0^{eq} + f_+^{eq} = \rho, \quad f_+^{eq} - f_-^{eq} = \rho u / c,$$

we have three equations (two linear and one nonlinear) for three unknowns. Expressing  $f_\pm^{eq}$  in terms of  $f_0^{eq}$ , and substituting these expressions into the detailed balance (5.16), we obtain a quadratic equation for  $f_0^{eq}$ ,

$$3(f_0^{eq})^2 - 8\rho f_0^{eq} + 4\rho^2 \left(1 - \frac{u^2}{c^2}\right) = 0,$$

whereupon the relevant solution reads

$$f_0^{\text{eq}} = \frac{2}{3}\rho \left( 2 - \sqrt{1 + \frac{3u^2}{c^2}} \right).$$

Introducing the speed of sound  $c_s = c/\sqrt{3}$ , we see that this expression is identical with the equilibrium of no-movers in (4.1). Same holds also for  $f_{\pm}^{\text{eq}}$ .

## 6 Admissible collision integrals

### 6.1 Admissibility conditions

Collision integrals in our geometric language are (column) vector-functions  $Q(f)$ . Collision integrals must respect three basic properties which we shall formulate now.

First,  $Q$  must be orthogonal to the hydrodynamic subspace  $\mathcal{H}^T$ ,

$$\text{if } h^T \in \mathcal{H}^T, \text{ then } h^T \cdot Q(f) = 0 \text{ for any } f. \quad (6.1)$$

By linearity, it is sufficient to require the orthogonality of  $Q$  with respect to any basis of the hydrodynamic space. In our case, we can require  $Q$  to be orthogonal to the basis row-vectors  $h_\rho^T$  and  $h_u^T$  (5.3),

$$h_\rho^T \cdot Q(f) = 0, \quad h_u^T \cdot Q(f) = 0 \text{ for any } f. \quad (6.2)$$

The requirement (6.1), or, equivalently, (6.2), is called *local conservation laws*, or (local) *invariants of the collision*. Local conservation laws in the construction of collision integrals always refer to the hydrodynamic fields (hence, to the basis row-vectors (5.3) in our case). It should be stressed at this point that  $Q$  should have *no* local conservation laws in the kinetic subspace. In our case this means,

$$\text{if } Q(f) \neq 0, \text{ then } k^T \cdot Q(f) \neq 0, \text{ for } k^T \in \mathcal{K}^T. \quad (6.3)$$

In brief, collision integral must respect the hydrodynamic local conservation laws and must have no other conservation laws.

The second requirement concerns the zero of the vector-function  $Q$ . Namely, the collision integral must be equal to zero (column-vectors with zero components) if and only if at the equilibrium,

$$Q(f) = 0 \text{ if and only if } f = f^{\text{eq}}. \quad (6.4)$$

Finally, the third basic requirement concerns the entropy production inequality. It states that the scalar product between the row-vector  $\nabla H^T$  (obtained by the transposition of the column-vector  $\nabla H$  (5.12)) at the state  $f$  and the row-vector  $Q$  at the same state is non-positive,

$$\sigma = \nabla H^T(f) \cdot Q(f) \leq 0, \text{ for any } f. \quad (6.5)$$



The equality sign in (6.5) should take place only at equilibrium (when  $f=f^{\text{eq}}$ ). In all other (*non-equilibrium*) states the entropy production must be strictly negative.

The three requirements (the local conservation laws (6.1), the zero of collisions (6.4), and the entropy production inequality (6.5)) must be met by any collision integral  $Q$ . Collision integrals which respect all these three requirements are called *admissible*. We leave it as an exercise to the reader to verify that the BGK collision integral (4.11) is admissible.

However, there are many more admissible collision integrals than just the BGK, and we shall now construct some of them for our discrete three-velocity model.

## 6.2 Gradient models

In this section we shall consider to families of admissible collision integrals. Both these families are constructed from the gradient of the entropy function,  $\nabla H$ , and we shall call them *gradient models*.

### 6.2.1 Family A gradient models

Let  $\Psi(z)$  be a function of one variable  $z$  (it is called *kinetic function*), which satisfies the following three properties:

$$\Psi(0)=0, \quad \Psi(z) \neq 0 \text{ if } z \neq 0, \quad z\Psi(z) \geq 0. \quad (6.6)$$

The collision integrals of the family A have the form:

$$Q = -\frac{1}{\tau} g \Psi(g^T \cdot \nabla H). \quad (6.7)$$

Here the factor  $1/\tau$  is introduced for a purpose of a later comparison to the BGK model. The rest of the construction follow the logic like this: Since we need to respect the local conservations,  $Q$  must be an element of the (row-vector) kinetic subspace  $\mathcal{K}$ . This motivates  $Q \propto g \Psi$  in (6.7). Next, the proportionality coefficient  $\Psi$  must vanish at the equilibrium (zero of collisions), so it must depend on the scalar product  $g^T \cdot \nabla H$  which is zero at the equilibrium (see the detailed balance condition (5.16)). Therefore, we come up with the first two requirements on the function  $\Psi$  (6.6). Finally, the third requirement in (6.6) guarantees the entropy production inequality (verify this!). Thus, all collision integrals of the family A are a admissible.

### 6.2.2 Family B gradient models

The construction is based on the stoichiometric representation of the column-vector  $g^T$  (5.10). Let  $\Phi(z)$  be again a function of one variable which satisfies the property of strict monotonicity,

$$\Phi(z_1) > \Phi(z_2) \text{ if } z_1 > z_2, \quad (6.8)$$

and which implies

$$(z_1 - z_2)(\Phi(z_1) - \Phi(z_2)) > 0 \text{ for any } z_1, z_2, z_1 \neq z_2 \quad (6.9)$$

Then the collision integrals of the family B have the form

$$Q = -\frac{1}{\tau} g \left( \Phi(g^{T+} \cdot \nabla H) - \Phi(g^{T-} \cdot \nabla H) \right). \quad (6.10)$$

The idea behind the collision integral (6.10) is much the same as for the family A:  $Q$  is proportional to  $g$ , while the proportionality coefficient is constructed upon rewriting the detailed balance condition (5.16) as

$$g^{T+} \cdot \nabla H|_{f_{\text{eq}}} = g^{T-} \cdot \nabla H|_{f_{\text{eq}}}. \quad (6.11)$$

Then the entropy production inequality becomes a simple implication of the monotonicity property (6.9),

$$\begin{aligned} \sigma &= -\frac{1}{\tau} \left( \nabla H^T \cdot g^+ - \nabla H^T \cdot g^- \right) \left( \Phi(g^{T+} \cdot \nabla H) - \Phi(g^{T-} \cdot \nabla H) \right) \\ &= -\frac{1}{\tau} \left( g^{T+} \cdot \nabla H - g^{T-} \cdot \nabla H \right) \left( \Phi(g^{T+} \cdot \nabla H) - \Phi(g^{T-} \cdot \nabla H) \right) \leq 0. \end{aligned} \quad (6.12)$$

Thus, all members of the family B are also admissible collision integrals.

The construction of the collision integrals of the families A and B requires the following ingredients: (i) Specification of the kinetic subspace (row-vector  $g^T$  in our case, and, in addition, the stoichiometric representation in the case of the family B), (ii) Specification of the entropy function  $H$  (function (3.17), and (iii) Specification of the kinetic function of one variable  $\Psi$  or  $\Phi$  with the properties (6.6) and (6.8), respectively. The key issue why the resulting collision integrals are admissible is in the detailed balance condition at the equilibrium. What is *not required* in the construction is the explicit form of the equilibrium (populations (4.1)). This is *the* difference between the BGK collision model (which *does* require the explicit form of the equilibrium). As we shall see it below, from the standpoint of reconstruction of the target Navier-Stokes equations all the models we discuss are equivalent.

Let us now finish the construction of the collision integrals (6.7) and (6.10). What remains to be done is to specify the kinetic functions  $\Psi$  and  $\Phi$ , and we shall consider the three most common choices.

*Linear function.* Function  $\Psi(z) = z$  satisfies (6.6), and the same function satisfies (6.8). In this case, family A and family B lead to the same collision integral

$$Q = -\frac{1}{\tau} g g^T \cdot \nabla H, \quad (6.13)$$

or, explicitly,

$$Q = -\frac{1}{\tau} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \ln \left( \frac{16f_- f_+}{f_0^2} \right). \quad (6.14)$$

Collision integrals of the form (6.14) will be called *gradient-A models*.

*Exponential function.* Function  $\Psi(z) = e^z - 1$  satisfies (6.6), and leads to the collision integral (6.7) of the form

$$Q = -\frac{1}{\tau} g \left( e^{g^T \cdot \nabla H} - 1 \right), \tag{6.15}$$

or, explicitly,

$$Q = -\frac{1}{\tau} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \left( \frac{16f_- f_+}{f_0^2} - 1 \right). \tag{6.16}$$

Collision integrals of the form (6.16) will be called *gradient-B models*.

The analog of this collision integral for the family B corresponds to the kinetic function  $\Phi(z) = e^z$ , which gives in (6.7)

$$Q = -\frac{1}{\tau} g \left( e^{g^{T+} \cdot \nabla H} - e^{g^{T-} \cdot \nabla H} \right), \tag{6.17}$$

or, explicitly,

$$Q = -\frac{1}{\tau} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} (16f_- f_+ - f_0^2). \tag{6.18}$$

Collision integrals of the form (6.18) are called *quasi-chemical models*. It is a place here to comment on this notion. Let us consider the populations as concentrations of some fictitious species  $A_-$ ,  $A_0$  and  $A_+$ , participating in a reversible ‘reaction’ with the following stoichiometric mechanism



In the direct reaction ( $\rightarrow$ ), one ‘molecule’ of  $A_-$  reacts with one ‘molecule’ of  $A_+$  to produce two ‘molecules’ of  $A_0$ . In the inverse reaction ( $\leftarrow$ ), two molecules of  $A_0$  produce one molecule of  $A_-$  and one molecule of  $A_+$ . Thus, the stoichiometry of the direct reaction is given by the row-vector,

$$g^{T+} = ( 1 \quad 0 \quad 1 ),$$

(participation of one molecule of  $A_-$  and one molecule of  $A_+$ ), and by the row-vector,

$$g^{T-} = ( 0 \quad 2 \quad 0 ),$$

for the reverse reaction (participation of two molecules of  $A_0$ ). These row-vectors are precisely the stoichiometric representation of the row-vector  $g^T$  (5.10). The rate of the reaction (6.19) can be constructed in the *mass action law* form. That is, the *gain rate* is proportional to the product  $w^+ f_- f_+$ , while the *loss rate* is proportional to  $w^- f_0 f_0$ . The ratio of the *equilibrium reaction constants*  $w^+ / w^-$  is dictated by the detailed balance condition (5.16), and is equal to 16 in our case. The total rate is thus written as ‘gain minus loss’ which leads to (6.18).

Table 1: Number of operations required to evaluate collision integrals.

Gradient-A (6.14)	45
Gradient-B (6.18)	5
Quasi-chemical (6.16)	6
BGK (4.11)	10

Thus, we have constructed several admissible collision integrals for the set of kinetic equations (4.10). As we shall see it in the next section, in spite of the fact that collision integrals (4.11), (6.14), (6.16) and (6.18) look rather different, they all lead to the same Navier-Stokes equations in the hydrodynamic limit. The idea about why this is so is quite simple: only the linearization of the collision integrals near equilibrium is relevant for the hydrodynamic limit, and the linear parts of all the collision integrals mentioned here are equivalent (warning: this is not so in higher dimensions!). On the other hand, these collision integrals are not equivalent in terms of their performance in the simulation. Indeed, they require not the same number of operations for their evaluation at a given state  $f$ . The most ‘expensive’ is the model (6.14) because it involves a logarithmic operation. On the other hand, the models (6.16) and (6.18) require even less operations than the BGK model. A comparison is given in Table 1 (where the logarithmic operation is estimated approximately as 40 operations).

In this section we have learned how to construct admissible collision integrals without knowing the equilibrium but only knowing the entropy function in the case when the kinetic subspace  $\mathcal{K}^T$  is one-dimensional (one basis row-vector  $g^T$ ).

We conclude this section with a generalizations of the Gradient-A collision integral to kinetic subspaces of any dimension. Let us consider a  $n_d$ -dimensional space of row-vectors  $\mathcal{E}^T$ , and its decomposition (5.11), where the dimension of the hydrodynamic subspace  $\mathcal{H}^T$  is  $n_c$  (the number of linearly independent conservation laws), and the dimension of the kinetic subspace  $\mathcal{K}^T$  is  $n_k = n_d - n_c$ . Let  $g_{(1)}^T, \dots, g_{(n_k)}^T$  be a basis (a maximal linearly independent system of row-vectors) of  $\mathcal{K}^T$ . Let  $H$  be a strictly convex function of the populations  $f_1, \dots, f_{n_d}$ , and  $\nabla H$  the column-vector of its partial derivatives. Let  $K$  be a positive-definite  $n_k \times n_k$  matrix with matrix elements  $K_{(s)(p)}$ ,  $s, p = 1, \dots, n_k$ . Then the following collision integral is obviously admissible:

$$Q = - \sum_{(s)=1}^{n_k} \sum_{(p)=1}^{n_k} g_{(s)} K_{(s)(p)} g_{(p)}^T \cdot \nabla H. \quad (6.20)$$

## 7 Linearization of collision integrals at equilibrium

### 7.1 Linearization of gradient models

When the populations become close to the (local) equilibrium, nonlinearity of the collision integrals becomes unimportant, and the relaxation at its final stages is governed by

the linearized collision integrals. In this section we shall collect the formulas of the linearized collision integrals of the previous section. They will be needed below to establish the hydrodynamic limit of the numerical schemes based on the minimal kinetic model.

We begin with the general formula of linearization for the collision integral of the family A (6.7). Substituting the population vector which slightly deviates from the equilibrium

$$f = f^{\text{eq}} + \delta f,$$

into (6.7), and retaining only the terms linear in  $\delta f$ , we obtain a perturbation of the collision integral (6.7) at equilibrium

$$Q(f^{\text{eq}}) + \delta Q = -\frac{1}{\tau} g \left[ \Psi \left( g^T \cdot \nabla H \Big|_{f^{\text{eq}}} \right) + \frac{d\Psi}{dz} \Big|_{z=g^T \cdot \nabla H \Big|_{f^{\text{eq}}}} g^T G(f^{\text{eq}}) \delta f \right]. \quad (7.1)$$

Here  $G$  is the matrix of second derivatives of the entropy function evaluated at the equilibrium,

$$G(f^{\text{eq}}) = \begin{pmatrix} \frac{1}{f_-^{\text{eq}}} & 0 & 0 \\ 0 & \frac{1}{f_0^{\text{eq}}} & 0 \\ 0 & 0 & \frac{1}{f_+^{\text{eq}}} \end{pmatrix}. \quad (7.2)$$

In this section, we shall not display the evaluation point  $f^{\text{eq}}$  in  $G$ , and write simply

$$G(f^{\text{eq}}) = G.$$

Thanks to the detailed balance (5.16), and to the properties of the kinetic function (6.6), we thus have in (7.1)

$$\delta Q = -\frac{1}{\tau} \Psi'(0) g g^T G \delta f, \quad (7.3)$$

where  $\Psi'(0)$  is the derivative of the kinetic function at  $z=0$ . Note that due to (6.6)  $\Psi'(0)$  is strictly positive.

Since (7.3) is valid for any  $\delta f \ll f^{\text{eq}}$ , we can write  $\delta Q$  (which is called *the differential* of the operator  $Q$  at equilibrium), in the form of the linear operator ( $3 \times 3$  matrix) acting on the column-vector  $\delta f$

$$\delta Q = L \delta f, \quad (7.4)$$

where

$$L = -\frac{1}{\tau} \Psi'(0) g g^T G \quad (7.5)$$

is called the *linearized collision integral* (or the Jacobian of the vector field  $Q$  at equilibrium). We leave it as an Exercise to obtain the explicit matrix form of the linearized collision integral (7.5) for the Gradient-A and Gradient-B models, (6.14) and (6.16).

Let us find the matrix  $L$  for the models (6.14) and (6.16). The derivative of the kinetic function  $\Psi(z) = z$  (Gradient-A model) at  $z=0$  is  $\Psi'(0) = 1$ , and the corresponding derivative of the function  $\Psi(z) = e^z - 1$  (Gradient-B model) is also  $\Psi'(0) = 1$ . Thus, the linearized collision integral (7.5) for both these models is the same,

$$L = -\frac{1}{\tau} g g^T G. \quad (7.6)$$

Furthermore,

$$g g^T = \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & -2 & 1 \end{pmatrix} = \begin{pmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{pmatrix}. \quad (7.7)$$

Multiplying this expression with the matrix  $G|_{f_{\text{eq}}}$ , we obtain

$$L = -\frac{1}{\tau} \begin{pmatrix} \frac{1}{f_-^{\text{eq}}} & -\frac{2}{f_0^{\text{eq}}} & \frac{1}{f_+^{\text{eq}}} \\ -\frac{2}{f_-^{\text{eq}}} & \frac{4}{f_0^{\text{eq}}} & -\frac{2}{f_+^{\text{eq}}} \\ \frac{1}{f_-^{\text{eq}}} & -\frac{2}{f_0^{\text{eq}}} & \frac{1}{f_+^{\text{eq}}} \end{pmatrix}. \quad (7.8)$$

Linearization of the collision integrals of the Family B (6.7) is much the same, and we shall write down the answer, leaving the derivation to the reader as an exercise:

$$L = -\frac{1}{\tau} \Phi' \left( g^{T+} \cdot \nabla H|_{f_{\text{eq}}} \right) g g^T G, \quad (7.9)$$

where the derivative of the kinetic function  $\Phi(z)$  is taken at  $z = g^{T+} \cdot \nabla H|_{f_{\text{eq}}}$ . By the detailed balance the latter value is also equal to  $g^{T-} \cdot \nabla H|_{f_{\text{eq}}}$ , thus, we can also write

$$L = -\frac{1}{\tau} \Phi' \left( g^{T-} \cdot \nabla H|_{f_{\text{eq}}} \right) g g^T G. \quad (7.10)$$

However, the most telling way to write the linearized collision integral for the Family B is the *symmetrized form* which is obtained by summing these two expressions and dividing by 2

$$L = -\frac{1}{2\tau} \left[ \Phi' \left( g^{T+} \cdot \nabla H|_{f_{\text{eq}}} \right) + \Phi' \left( g^{T-} \cdot \nabla H|_{f_{\text{eq}}} \right) \right] g g^T G. \quad (7.11)$$

Let us find the matrix  $L$  (7.11) for the quasi-chemical collision integral (6.18). Evaluating the derivative of the kinetic function  $\Phi(z) = e^z$  at  $z = g^{T\pm} \cdot \nabla H|_{f_{\text{eq}}}$ , and using the result of the previous Exercise, we find

$$L = -\frac{1}{2\tau} (16f_-^{\text{eq}} f_+^{\text{eq}} + f_0^{\text{eq}} f_0^{\text{eq}}) \begin{pmatrix} \frac{1}{f_-^{\text{eq}}} & -\frac{2}{f_0^{\text{eq}}} & \frac{1}{f_+^{\text{eq}}} \\ -\frac{2}{f_-^{\text{eq}}} & \frac{4}{f_0^{\text{eq}}} & -\frac{2}{f_+^{\text{eq}}} \\ \frac{1}{f_-^{\text{eq}}} & -\frac{2}{f_0^{\text{eq}}} & \frac{1}{f_+^{\text{eq}}} \end{pmatrix}. \quad (7.12)$$

We shall postpone the discussion of the properties of the linearized gradient collision integrals to the end of this section, and will consider first the linearization of the BGK operator.

## 7.2 Linearized BGK operator and thermodynamic projector

Let us turn to the linearization of the BGK collision integral (4.11). We write

$$\delta Q = -\frac{1}{\tau} \left( \delta f - \frac{\partial f^{\text{eq}}}{\partial \rho} \delta \rho - \frac{\partial f^{\text{eq}}}{\partial u} \delta u \right). \quad (7.13)$$

Now we shall use the fact that the variation of the density  $\rho$  and of the velocity  $u$  are written as scalar products between the column-vector  $\delta f$  and the row-vectors of the hydrodynamic subspace

$$\begin{aligned} \delta \rho &= h_\rho^T \cdot \delta f, \\ \delta u &= \frac{c}{\rho} \left( h_u^T \cdot \delta f \right) - \frac{u}{\rho} \left( h_\rho^T \cdot \delta f \right). \end{aligned} \quad (7.14)$$

With this, the linearized collision integral of the BGK is written as

$$L = -\frac{1}{\tau} (1 - P) \delta f, \quad (7.15)$$

where 1 is the unit matrix, and  $P$  is a projector (this is the simplest instance of the *thermodynamic projector* [22])

$$P = \left( \frac{\partial f^{\text{eq}}}{\partial \rho} - \frac{u}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) h_\rho^T + \left( \frac{c}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) h_u^T. \quad (7.16)$$

Operator  $P$  is called projector if its repeated action on any vector  $\delta f$  equals the action of  $P$ , or

$$PP = P. \quad (7.17)$$

Let us verify that the operator  $P$  (7.16) satisfies the projector property (7.17):

$$\begin{aligned} PP\delta f &= \left( \frac{\partial f^{\text{eq}}}{\partial \rho} - \frac{u}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) \left[ \left( h_\rho^T \cdot \left( \frac{\partial f^{\text{eq}}}{\partial \rho} - \frac{u}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) \right) (h_\rho^T \cdot \delta f) + \frac{c}{\rho} \left( h_\rho^T \cdot \frac{\partial f^{\text{eq}}}{\partial u} \right) (h_u^T \cdot \delta f) \right] \\ &+ \left( \frac{c}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) \left[ \left( h_u^T \cdot \left( \frac{\partial f^{\text{eq}}}{\partial \rho} - \frac{u}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) \right) (h_\rho^T \cdot \delta f) + \frac{c}{\rho} \left( h_u^T \cdot \frac{\partial f^{\text{eq}}}{\partial u} \right) (h_u^T \cdot \delta f) \right]. \end{aligned} \quad (7.18)$$

Evaluating scalar products in this expression, we have

$$\begin{aligned} \left( h_\rho^T \cdot \left( \frac{\partial f^{\text{eq}}}{\partial \rho} - \frac{u}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) \right) &= \frac{\partial \rho}{\partial \rho} - \frac{u}{\rho} \frac{\partial \rho}{\partial u} = 1, \\ \left( h_\rho^T \cdot \frac{\partial f^{\text{eq}}}{\partial u} \right) &= \frac{\partial \rho}{\partial u} = 0, \\ \left( h_u^T \cdot \left( \frac{\partial f^{\text{eq}}}{\partial \rho} - \frac{u}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) \right) &= \frac{1}{c} \frac{\partial(\rho u)}{\partial \rho} - \frac{u}{c\rho} \frac{\partial(\rho u)}{\partial u} = 0, \\ \frac{c}{\rho} \left( h_u^T \cdot \frac{\partial f^{\text{eq}}}{\partial u} \right) &= \frac{1}{\rho} \frac{\partial(\rho u)}{\partial u} = 1. \end{aligned} \quad (7.19)$$

Substituting these expressions into (7.18), we continue the computation of  $PP\delta f$ ,

$$\begin{aligned} PP\delta f &= \left( \frac{\partial f^{\text{eq}}}{\partial \rho} - \frac{u}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) (h_\rho^T \cdot \delta f) + \left( \frac{c}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) (h_u^T \cdot \delta f) \\ &= P \cdot \delta f. \end{aligned} \quad (7.20)$$

Since  $\delta f$  was arbitrary in this computation, we have proven the projector property (7.17). Because operator  $P$  is a projector, then operator  $1 - P$  is also a projector,

$$(1 - P)(1 - P) = 1 - 2P + PP = 1 - P. \quad (7.21)$$

Thus, the linearized BGK operator is just proportional to the projector  $1 - P$ . Properties of the projectors  $P$  and  $1 - P$  are so much important that we shall discuss them here in some detail.

We first remind that two linear subspaces, denoted as  $\text{im}P$  (the image of  $P$ ) and  $\text{ker}P$  (the kernel of  $P$ ) are associated with any projector. Each vector of the kernel is annihilated by the projector,  $Pf = 0$  if  $f \in \text{ker}P$ . Vectors of image of the projector satisfy the condition  $Pf = f$ . The kernel of projector  $P$  (7.16) is the kinetic subspace  $\mathcal{K}$ ,

$$\text{ker}P = \mathcal{K}. \quad (7.22)$$

For the projector  $1 - P$ , the situation is opposite,

$$\text{im}(1 - P) = \mathcal{K}. \quad (7.23)$$

The proof of (7.22) (and, accordingly, of (7.23)) follows from the definitions of the subspace  $\mathcal{K}$ : any vector of the kinetic subspace  $\mathcal{K}$  has the form  $ag$ , so

$$Pag = a \left( \frac{\partial f^{\text{eq}}}{\partial \rho} - \frac{u}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) (h_\rho^T \cdot g) + a \left( \frac{c}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) (h_u^T \cdot g) = 0. \quad (7.24)$$

Thus, any vector of  $\mathcal{K}$  is annihilated by  $P$ . On the other hand, for any nontrivial vector  $h$  from the hydrodynamic subspace, either  $h_\rho^T \cdot h \neq 0$  or  $h_u^T \cdot h \neq 0$  (certainly, these quantities can be both non-zero), thus,  $Ph \neq 0$  for any  $h \in \mathcal{H}$ . Since any vector can be represented as  $ag + h$  with some  $a$  and some  $h \in \mathcal{H}$ , we have proven (7.22). The proof of (7.23) follows from the fact that  $(1 - P)ag = ag$ .

The dimension of the subspace  $\text{im}P$  is  $\dim(\text{im}P) = n_d - \dim(\text{ker}P)$ , in our case  $\dim \text{im}P = 2$  (thus,  $\dim(\text{ker}(1 - P)) = n_d - \dim(\text{im}(1 - P))$ , in our case  $\dim \text{ker}(1 - P) = 1$ ). The image of  $P$  (7.16) is a linear subspace spanned by the two column-vectors,

$$e_\rho = \frac{\partial f^{\text{eq}}}{\partial \rho}, \quad e_u = \frac{\partial f^{\text{eq}}}{\partial u}. \quad (7.25)$$

That is,

$$\text{im}P = \{ \text{All vectors of the form } ae_\rho + be_u \}. \quad (7.26)$$



In order to prove this statement, we need to show that

$$P(ae_\rho + be_u) = ae_\rho + be_u,$$

for any coefficients  $a$  and  $b$ . This is achieved by a direct computation

$$\begin{aligned} & P(ae_\rho + be_u) \\ &= \left( \frac{\partial f^{\text{eq}}}{\partial \rho} - \frac{u}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) \left( h_\rho^T \cdot \left( a \frac{\partial f^{\text{eq}}}{\partial \rho} + b \frac{\partial f^{\text{eq}}}{\partial u} \right) \right) + \frac{1}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \left( ch_u^T \cdot \left( a \frac{\partial f^{\text{eq}}}{\partial \rho} + b \frac{\partial f^{\text{eq}}}{\partial u} \right) \right) \\ &= \left( \frac{\partial f^{\text{eq}}}{\partial \rho} - \frac{u}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) \left( a \frac{\partial \rho}{\partial \rho} + b \frac{\partial \rho}{\partial u} \right) + \frac{1}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \left( a \frac{\partial(\rho u)}{\partial \rho} + b \frac{\partial(\rho u)}{\partial u} \right) \\ &= \left( \frac{\partial f^{\text{eq}}}{\partial \rho} - \frac{u}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} \right) a + \frac{1}{\rho} \frac{\partial f^{\text{eq}}}{\partial u} (au + b\rho) \\ &= a \frac{\partial f^{\text{eq}}}{\partial \rho} + b \frac{\partial f^{\text{eq}}}{\partial u} = ae_\rho + be_u. \end{aligned} \tag{7.27}$$

The image of the projector  $P$  has the following geometric interpretation. The set of the equilibrium populations can be viewed as two-dimensional *sub-manifold* (a surface) in the three-dimensional space of populations. This sub-manifold is parameterized by two parameters,  $\rho$  and  $u$ . The *tangent space* to this sub-manifold at the point  $f^{\text{eq}}(\rho, u)$  is the linear hull of the two partial derivatives,  $\partial f^{\text{eq}}(\rho, u)/\partial \rho$  and  $\partial f^{\text{eq}}(\rho, u)/\partial u$ . These derivatives are precisely the vectors  $e_\rho$  and  $e_u$  (7.25), and the tangent space to the equilibrium sub-manifold at the point with the coordinates  $(\rho, u)$  is the image of the projector  $P$  (7.16). Put differently, we can say that  $P$  projects onto the tangent space of the equilibrium sub-manifold ( $\text{im}P$ ), and parallel to the kinetic subspace ( $\text{ker}P$ ). For the projector  $1 - P$ , the situation is opposite, it projects onto the kinetic subspace parallel to the tangent space. All projections are understood locally, that is, the tangent space is different at different points on the sub-manifold.

A one more question which one typically needs to answer when considering a projector is about *orthogonality*. When speaking of orthogonality, one refers to a scalar product. Above, we have considered the orthogonality of the kinetic and the hydrodynamic subspaces *with respect to the standard scalar product*  $\cdot$  (5.2). Orthogonality of projector  $P$  with respect to a specified scalar product  $*$  means that every vector of the kernel is orthogonal to any vector of the image in the sense of  $*$ . Is the projector  $P$  in (7.16) orthogonal with respect to the standard scalar product  $\cdot$ ? The answer is *negative*, it is *not* orthogonal with respect to this scalar product, the image of the projector  $P$  has the components in both the kinetic and the hydrodynamic subspaces. In order to show this, it is sufficient to find a non-trivial pair of vectors, one from the kernel of  $P$  and another from the image of  $P$  such that their standard scalar product is not equal to zero. For example, let us consider the vector  $e_\rho$  (7.25) at the zero-velocity equilibrium  $f^{\text{eq}}(\rho, 0)$ . Let us find the standard scalar product between this vector and the vector  $g$ . From (4.1) we have

$$e_\rho(0) = \frac{\partial f^{\text{eq}}(\rho, u)}{\partial \rho} \Big|_{u=0} = \left( \frac{1}{6} \quad \frac{4}{6} \quad \frac{1}{6} \right)^T. \tag{7.28}$$

It follows from (5.8) that

$$g^T \cdot e_\rho(0) = -1 \neq 0. \quad (7.29)$$

However, there exists another scalar product relative to which  $P$  is orthogonal. This scalar product is called the *entropic scalar product*, and it is constructed with the help of the positive-definite matrix of the second derivatives of the entropy function. In our case this is the matrix  $G$  given by (7.2). We shall denote  $*$  the entropic scalar product between vectors  $e$  and  $f$ ,

$$e^T * f = f^T * e = e^T \cdot G \cdot f = \frac{e_- f_-}{f_-^{\text{eq}}} + \frac{e_0 f_0}{f_0^{\text{eq}}} + \frac{e_+ f_+}{f_+^{\text{eq}}}. \quad (7.30)$$

Orthogonality of  $P$  with respect to  $*$  (7.30) means

$$((1-P)e)^T * Pf = 0 \quad (7.31)$$

for any pair of vectors  $e, f$ . In order to demonstrate this in our case, it is sufficient to prove that

$$g^T * (ae_\rho + be_u) = 0. \quad (7.32)$$

Indeed, the vectors of the kernel of  $P$  are proportional to vector  $g$ , while all vectors of the image of  $P$  have the form (7.26), so equality (7.32) implies orthogonality of  $P$  with respect to the entropic scalar product. Verification of (7.32) is done upon a direct computation. We shall do this computation without even a reference to the specific entropy function of our example in order to stress generality.

Since  $a$  and  $b$  are arbitrary in (7.32), it is sufficient to prove that

$$g^T * \left( \frac{\partial f^{\text{eq}}}{\partial \rho} \right) = 0, \quad g^T * \left( \frac{\partial f^{\text{eq}}}{\partial u} \right) = 0. \quad (7.33)$$

Computing the first of these expressions, we have

$$\begin{aligned} g^T * \left( \frac{\partial f^{\text{eq}}}{\partial \rho} \right) &= g^T \cdot G \frac{\partial f^{\text{eq}}}{\partial \rho} \\ &= g^T \cdot \left( \frac{\partial \nabla H|_{f^{\text{eq}}}}{\partial \rho} \right) = \frac{\partial (g^T \cdot \nabla H|_{f^{\text{eq}}})}{\partial \rho} = 0. \end{aligned} \quad (7.34)$$

In the last line of the computation we have again used the detailed balance condition (5.16). Computation of the second of the scalar products in (7.33) is done in just the same way. Since the scalar product in (7.32) is a linear combination of the products (7.33), we have proven the orthogonality of  $P$  with respect to the entropic scalar product. We see that the orthogonality of  $P$  is the implication of the detail balance in every point of the equilibrium manifold  $f^{\text{eq}}(\rho, u)$ .

Let us prove, as an example, the orthogonality (7.32) for the Boltzmann entropy function

$$H = \sum_{i=1}^{n_d} f_i \ln \left( \frac{f_i}{W_i} \right).$$

(For the  $H$ -function (3.17),  $W_{\pm} = 1$ ,  $W_0 = 4$ ). Indeed,

$$\begin{aligned}
 g^T * (ae_{\rho} + be_u) &= \sum_{i=1}^{n_d} \frac{g_i}{f_i^{\text{eq}}} \left( a \frac{\partial f_i^{\text{eq}}}{\partial \rho} + b \frac{\partial f_i^{\text{eq}}}{\partial u} \right) \\
 &= \sum_{i=1}^{n_d} g_i \left( a \frac{\partial \ln f_i^{\text{eq}}}{\partial \rho} + b \frac{\partial \ln f_i^{\text{eq}}}{\partial u} \right) \\
 &= \sum_{i=1}^{n_d} g_i \left( a \frac{\partial (\ln(f_i^{\text{eq}}/W_i) + \ln W_i)}{\partial \rho} + b \frac{\partial (\ln(f_i^{\text{eq}}/W_i) + \ln W_i)}{\partial u} \right) \\
 &= a \frac{\partial (g^T \cdot \nabla H|_{f^{\text{eq}}})}{\partial \rho} + b \frac{\partial (g^T \cdot \nabla H|_{f^{\text{eq}}})}{\partial u} \\
 &= 0.
 \end{aligned} \tag{7.35}$$

Thus,  $P$  projects orthogonally with respect to the entropic scalar product. The immediate consequence of this is that  $P$  is self-adjoint (in the same, entropic scalar product sense). Operator (matrix)  $A^{\dagger}$  is called adjoint to operator  $A$ , if for any two vectors  $e$  and  $f$  we have

$$e^T * (Af) = f^T * (A^{\dagger}e). \tag{7.36}$$

Note again that specification of the scalar product is required when talking about adjoint operators. Operator  $A$  is called self-adjoint (with respect to  $*$ ) if

$$A^{\dagger} = A. \tag{7.37}$$

Orthogonal projectors are also self-adjoint (the inverse of this statement is also true). Thus, projector  $P$  (7.16) (and also projector  $1 - P$ ) is self-adjoint in the entropic scalar product

$$P^{\dagger} = P, \quad (1 - P)^{\dagger} = (1 - P). \tag{7.38}$$

We suggest the reader to prove this statement as an exercise.

From all the above discussion we conclude that the linearized BGK operator is proportional to the orthogonal projector  $1 - P$ , and we have described this operator completely (that is, we know its kernel and image). Thus, we also know the complete solution to the eigenvalue problem for this operator,

$$L\delta f = \lambda\delta f. \tag{7.39}$$

There are two eigenvalues for this problem,  $\lambda_0 = 0$  and  $\lambda = -1/\tau$ . The eigenspace corresponding to the zero eigenvalue  $\lambda_0$  is twice degenerated, and corresponds to the two-dimensional image of the projector  $P$ . The eigenspace corresponding to  $\lambda$  is spanned by the kinetic vector  $g$ , and corresponds to the kernel of  $P$ . These eigenspaces are orthogonal to each other in the sense of the entropic scalar product. Operator  $L$  is self-adjoint with

respect to the entropic scalar product, and, moreover, is non-positive definite. The latter means that,

$$(\delta f)^T * (L\delta f) \leq 0 \quad \text{for any } \delta f, \tag{7.40}$$

and we leave it to the reader to verify this inequality.

### 7.3 Thermodynamic projector in canonic form

Let us come back to the discussion of properties of the linearized operators (7.5) and (7.11). These operators differ only by a factor (which nevertheless may depend on  $f^{\text{eq}}$ ), so we consider a general form

$$L = -\frac{1}{\tau} k g g^T G, \tag{7.41}$$

where the positive factor  $k$  takes the following values

$$\begin{aligned} k &= \Psi'(0) \quad \text{for (7.5),} \\ k &= \frac{1}{2} \left[ \Phi'(g^{T+} \cdot \nabla H|_{f^{\text{eq}}}) + \Phi'(g^{T-} \cdot \nabla H|_{f^{\text{eq}}}) \right] \quad \text{for (7.11).} \end{aligned} \tag{7.42}$$

In order to find out the properties of the operator  $L$  (7.41), and to compare it with the linearized BGK operator, it proves instructive to rewrite (7.41) as follows:

$$L = -\frac{1}{\tau} k (g^T * g) (1 - \Pi), \tag{7.43}$$

where we have used the above notation for the entropic scalar product ( $\sqrt{g^T * g}$  can be termed the entropic norm of the kinetic vector  $g$  at equilibrium), and we have introduced operator  $\Pi$

$$\Pi = 1 - \frac{1}{(g^T * g)} g g^T G. \tag{7.44}$$

It is easy to prove that  $\Pi$  is again a projector:

$$\begin{aligned} \Pi \Pi &= \left( 1 - \frac{g g^T G}{(g^T * g)} \right) \left( 1 - \frac{g g^T G}{(g^T * g)} \right) \\ &= 1 - 2 \frac{g g^T G}{(g^T * g)} + \frac{g (g^T \cdot G g) g^T G}{(g^T * g)^2} \\ &= \Pi. \end{aligned} \tag{7.45}$$

The kernel of the projector  $\Pi$  is again the kinetic subspace,

$$\ker \Pi = \mathcal{K}. \tag{7.46}$$

This is verified immediately:

$$\Pi g = g - g \frac{(g^T \cdot G g)}{(g^T * g)} = g - g = 0. \tag{7.47}$$

By looking at our previous result for the thermodynamic projector  $P$ , Eq. (7.22), we notice that  $\Pi$  and  $P$  have identical kernels,

$$\ker \Pi = \ker P. \tag{7.48}$$

However, the form of  $\Pi$  (7.44) does not look much similar to  $P$  (7.16). Nevertheless, projector  $\Pi$  is the same thermodynamic projector! This means, that also the image of  $\Pi$  is the tangent space to the equilibrium manifold. Indeed, we can compute the action of  $\Pi$  on any vector from  $\text{im}P$  (7.26) to see that  $\Pi$  leave invariant such vectors:

$$\begin{aligned} \Pi(ae_\rho + be_u) &= a \left( e_\rho - \frac{g(g^T * e_\rho)}{(g^T * g)} \right) + b \left( e_u - \frac{g(g^T * e_u)}{(g^T * g)} \right) \\ &= ae_\rho + be_u, \end{aligned} \tag{7.49}$$

and this proves

$$\text{im} \Pi = \text{im} P. \tag{7.50}$$

Two projectors  $P_1$  and  $P_2$  with identical kernels and identical images are *equivalent* (one writes  $P_1 \sim P_2$ ). Projectors  $\Pi$  (7.44) and  $P$  (7.16) have the same kernel and the same image, so they are equivalent,

$$\Pi \equiv P. \tag{7.51}$$

Projector  $\Pi$  is therefore called *thermodynamic projector in canonic form*. Note that while we needed to compute derivatives of the equilibrium populations  $f^{\text{eq}}(\rho, u)$  when writing the thermodynamic projector  $P$  (7.16), we did not need anything like that when writing its canonic form  $\Pi$ . In other words,  $\Pi$  is just the orthogonal (in the  $*$ -sense) projector with the kernel  $\mathcal{K}$ .

One more interesting observation can be made here. Suppose we were not knowing anything about the thermodynamic projector  $P$  (7.16). Then we would still have found the image of  $\Pi$  quite easily: let us consider any vector  $h$  of the hydrodynamic subspace  $\mathcal{H}$ , and transform it with the inverse operator  $G^{-1}$ . This transformed vector  $\tilde{h}$ ,

$$\tilde{h} = G^{-1}h, \tag{7.52}$$

is a vector of the image of  $\Pi$ :

$$\Pi \tilde{h} = \tilde{h} - \frac{g g^T G G^{-1} h}{(g^T * g)} = \tilde{h} - \frac{g(g^T \cdot h)}{(g^T * g)} = \tilde{h}, \tag{7.53}$$

by the orthogonality (with respect to  $\cdot$ ) of kinetic and hydrodynamic subspaces. Thus, the image of  $\Pi$  is also described as a linear transformation of the hydrodynamic subspace

$$\text{im} \Pi = G^{-1} \mathcal{H}. \tag{7.54}$$

But thanks to equivalence of  $P$  and  $\Pi$  the linear subspace  $G^{-1} \mathcal{H}$  must be the same thing as  $\text{im}P$  (7.26). Both representations of  $\text{im} \Pi$  (or of  $\text{im}P$ ) can be now compared, that is, there

must be a non-degenerated linear transformation which transforms vectors of the form  $G^{-1}h$  (7.52) into vectors of the form  $ae_\rho + be_u$ . Let us find this transformation explicitly. We write, using the fact that  $\nabla H$  at equilibrium is a linear combination of the vectors  $h_\rho$  and  $h_u$

$$\begin{aligned} G(ae_\rho + be_u) &= a \frac{\partial \nabla H|_{f^{\text{eq}}}}{\partial \rho} + b \frac{\partial \nabla H|_{f^{\text{eq}}}}{\partial u} \\ &= a \left( h_\rho \frac{\partial \chi}{\partial \rho} + h_u c \frac{\partial \lambda}{\partial \rho} \right) + b \left( h_\rho \frac{\partial \chi}{\partial u} + h_u c \frac{\partial \lambda}{\partial u} \right) \\ &= \tilde{a} h_\rho + \tilde{b} h_u, \end{aligned} \quad (7.55)$$

where

$$\tilde{a} = a \frac{\partial \chi}{\partial \rho} + b \frac{\partial \chi}{\partial u}, \quad \tilde{b} = ac \frac{\partial \lambda}{\partial \rho} + bc \frac{\partial \lambda}{\partial u}, \quad (7.56)$$

or, in a matrix form,

$$\begin{pmatrix} \tilde{a} \\ \tilde{b} \end{pmatrix} = \begin{pmatrix} \frac{\partial \chi}{\partial \rho} & \frac{\partial \chi}{\partial u} \\ c \frac{\partial \lambda}{\partial \rho} & c \frac{\partial \lambda}{\partial u} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}. \quad (7.57)$$

Eq. (7.57) establishes the relation between the two representations of the image of the thermodynamic projector, (7.26) and (7.54). In order that this relation be one-into-one, the matrix  $D$  (which has the dimension  $n_c \times n_c$ , where  $n_c$  is the number of conservation laws,  $2 \times 2$  in our case),

$$D = \begin{pmatrix} \frac{\partial \chi}{\partial \rho} & \frac{\partial \chi}{\partial u} \\ c \frac{\partial \lambda}{\partial \rho} & c \frac{\partial \lambda}{\partial u} \end{pmatrix}, \quad (7.58)$$

must be non-degenerated,

$$\det D = c \left( \frac{\partial \chi}{\partial \rho} \right) \left( \frac{\partial \lambda}{\partial u} \right) - c \left( \frac{\partial \chi}{\partial u} \right) \left( \frac{\partial \lambda}{\partial \rho} \right) \neq 0. \quad (7.59)$$

Matrix  $D$  is the Jacobian of the map of Lagrange multipliers,  $\chi$  and  $\lambda$ , into the hydrodynamic variables,  $\rho$  and  $u$ . The non-degeneracy condition (7.59) tells that the coordinates  $\rho$  and  $u$  distinguish points on the equilibrium manifold  $f^{\text{eq}}(\rho, u)$ , two different pairs of values,  $(\rho_1, u_1)$  and  $(\rho_2, u_2)$ , correspond to two different equilibria,  $f^{\text{eq}}(\rho_1, u_1)$  and  $f^{\text{eq}}(\rho_2, u_2)$ . Condition (7.59) is called *transversality condition*. It is straightforward to verify that the equilibrium (4.1) satisfies the transversality condition (7.59).

The linearized collision integral (7.41) is just proportional to the same projector  $1 - P$  as the linearized BGK, hence, the properties of (7.41) are also much the same. The difference is that the proportionality coefficient  $K(g^T * g)$  can depend on the equilibrium populations, and thus be a function of  $\rho$  and  $u$ . The spectrum of the operator (7.41) consists of two eigenvalues: the twice degenerated  $\lambda_0 = 0$  and  $\lambda = -\frac{1}{\tau} k(g^T * g)$ . Unlike the case of the BGK model, the latter eigenvalue can be a function of  $\rho$  and  $u$ . A small modification of gradient models is required if we want their linearization to be *exactly* as the linearized BGK.

## 8 Single relaxation time gradient models

As we can infer from the above remarks, one needs to compensate for the “extra” factor (7.41) by dividing the collision integral with  $k(g^T * g)$ . Let us do this “division” carefully for the Family A, where  $k = \Psi'(0)$  is a constant (even then we still have the dependence of the eigenvalue  $\lambda$  on  $\rho$  and  $u$  entering through the entropic scalar product  $g^T * g$  at equilibrium). Let us begin with a slight generalization of the gradient models, and will spell out all the dependencies on the populations in all the expressions (though a bit bulky, this is needed in order to avoid confusion).

$$Q(f) = -\frac{1}{\tau} K(f) g \Psi \left( g^T \cdot \nabla H \right), \quad (8.1)$$

where we have introduced a yet undefined positive function of populations  $K(f)$ . Obviously, all collision integrals (8.1) are admissible. Linearization of (8.1) gives

$$\begin{aligned} Q(f^{\text{eq}}) + \delta Q = & -\frac{1}{\tau} K(f^{\text{eq}}) g \Psi(0) - \frac{1}{\tau} K(f^{\text{eq}}) \Psi'(0) g g^T G(f^{\text{eq}}) \delta f \\ & - \frac{1}{\tau} (\nabla K^T(f^{\text{eq}}) \cdot \delta f) g \Psi(0), \end{aligned} \quad (8.2)$$

where  $\nabla K^T(f^{\text{eq}})$  is the row-vector of the partial derivatives of the function  $K$  at the equilibrium. The first and the last terms in this expression vanish<sup>‡</sup>, and we thus have for the linearized collision integral

$$L = -\frac{1}{\tau} K(f^{\text{eq}}) \Psi'(0) g g^T G(f^{\text{eq}}), \quad (8.3)$$

or, using the results of the previous section, and spelling out the entropic scalar product  $g^T * g$ ,

$$L = -\frac{1}{\tau} \left( K(f^{\text{eq}}) \Psi'(0) g^T \cdot (G(f^{\text{eq}}) g) \right) (1 - \Pi). \quad (8.4)$$

We see that the *single relaxation time condition* requires

$$K(f^{\text{eq}}) \Psi'(0) g^T \cdot (G(f^{\text{eq}}) g) = 1, \quad (8.5)$$

or

$$K(f^{\text{eq}}) = \frac{1}{\Psi'(0) g^T \cdot (G(f^{\text{eq}}) g)}. \quad (8.6)$$

We see that the condition (8.6) is the only requirement on the function  $K$  which, once satisfied, makes the linearized collision integral just as the linearized BGK. One obvious way to achieve this is to set

$$K(f) = K(f^{\text{eq}}(\rho(f), u(f))) = \frac{1}{g^T \cdot (G(f^{\text{eq}}) g) \Psi'(0)}, \quad (8.7)$$

<sup>‡</sup>If  $Q$  is admissible collision integral, then  $\delta(KQ) = \delta K Q(f^{\text{eq}}) + K(f^{\text{eq}}) \delta Q = K(f^{\text{eq}}) \delta Q$ .

in (8.1). In other words, we can *define* the function of populations  $K(f)$  as in (8.7), and use the gradient model

$$Q = -\frac{1}{\tau} \left( \frac{1}{g^T \cdot (G(f^{eq})g)\Psi'(0)} \right) g \Psi(g^T \cdot \nabla H), \tag{8.8}$$

which is then equivalent to the BGK in the linear approximation.

However, this is not yet a very interesting suggestion from the practical standpoint because the equilibrium population needs to be known explicitly for writing up (8.7). A more interesting model is established upon extending the single relaxation time condition (8.6) from equilibrium onto all other states. That is, instead of (8.7), we define the function  $K$  as

$$K(f) = \frac{1}{g^T \cdot G(f)g\Psi'(0)}. \tag{8.9}$$

Here the denominator in the right hand side contains the entropic scalar product in the state  $f$  (rather than in the equilibrium). In order to stress this fact, we write

$$g^T *_f g = g^T \cdot G(f)g = \frac{1}{f_-} + \frac{4}{f_0} + \frac{1}{f_+}. \tag{8.10}$$

With the choice (8.9), the *single relaxation time model* (SRTM) within the Family A is written as

$$Q = -\frac{1}{\tau} \left( \frac{1}{g^T *_f g\Psi'(0)} \right) g \Psi(g^T \cdot \nabla H). \tag{8.11}$$

For the linear and for the exponential functions  $\Psi$  considered in Section 6.2,  $\Psi'(0) = 1$ , and we list here the corresponding SRTM modifications of them. The SRTM gradient-A model (see (6.13)) reads,

$$Q = -\frac{1}{\tau} (g^T *_f g)^{-1} g g^T \cdot \nabla H, \tag{8.12}$$

or, explicitly (see (6.14)),

$$Q = -\frac{1}{\tau} \left( \frac{1}{f_-} + \frac{4}{f_0} + \frac{1}{f_+} \right)^{-1} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \ln \left( \frac{16f_- f_+}{f_0^2} \right). \tag{8.13}$$

The SRTM gradient-B model reads,

$$Q = -\frac{1}{\tau} (g^T *_f g)^{-1} g \left( e^{g^T \cdot \nabla H} - 1 \right), \tag{8.14}$$

or, explicitly (see (6.16)),

$$Q = -\frac{1}{\tau} \left( \frac{1}{f_-} + \frac{4}{f_0} + \frac{1}{f_+} \right)^{-1} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \left( \frac{16f_- f_+}{f_0^2} - 1 \right). \tag{8.15}$$



The SRTM collision integrals (8.13) and (8.15) have the following properties: *They do not require the equilibrium to be evaluated explicitly, and, at the same time, their linearization around equilibrium is the same operator, as it is for the BGK model.*

We conclude this section by writing down a SRTM Gradient-A model for a multi-dimensional case. In order to do this, we choose the  $n_k \times n_k$  matrix  $K$  in (6.20) as follows [14]:

$$K = C^{-1}, \quad (8.16)$$

where  $C$  is the *correlation matrix* with the components

$$C_{(s)(p)} = \sum_{i=1}^{n_d} \sum_{j=1}^{n_d} g_{(s)i} \frac{\partial^2 H}{\partial f_i \partial f_j} g_{(p)j}. \quad (8.17)$$

## 9 Entropic lattice Boltzmann scheme

### 9.1 Hydrodynamic limit in the discrete-time picture

With the results derived above (the entropy function, the equilibrium, and a set of admissible single relaxation time collision integrals), we are in a position now to derive the entropic lattice Boltzmann scheme for the present model. Since the principles of construction of the entropic scheme were discussed in detail in the previous paper [1], we here present only the resulting formulas. Populations are updated according to the fully discrete kinetic equation,

$$f_i(x + c_i \delta t, t + \delta t) - f_i(x, t) = Q_i^*(f(x, t)), \quad (9.1)$$

where  $Q^*$  is *dressed* (or *stabilized*) single relaxation time collision integral,

$$Q^* = \beta \alpha Q. \quad (9.2)$$

Here  $\beta \in [0, 1]$  is a parameter related to viscosity (see (9.36) below), and  $\alpha$  is the scalar function of the population vector. Function  $\alpha$  ensures the discrete-time  $H$ -theorem, and is the nontrivial root of the scalar nonlinear equation,

$$H(f) = H(f + \alpha Q(f)). \quad (9.3)$$

Put differently, collision integrals are merely directions in the space of populations, pointing towards the change of the state during the collision step. Parameter  $\alpha$  defines the maximal admissible collision step along this direction so that the entropy will not decrease. The combination  $\beta \alpha$  is thus the effective relaxation parameter in the fully discrete kinetic picture.

Identification of the viscosity coefficient in the entropic lattice Boltzmann method is done on the basis of the Chapman-Enskog analysis in the vicinity of the local equilibrium. Let us consider this derivation in some detail below. Before so doing, we shall consider linearization of dressed collision integral (9.2) for single relaxation time models.

## 9.2 Linearization of dressed collision integrals

Linearization of the dressed collision integral (9.2) may be written as,

$$\delta Q_i^* = \beta \alpha(f^{\text{eq}}) \left( \sum_{j=1}^{n_d} \frac{\partial Q_j}{\partial f_j} \Big|_{f^{\text{eq}}} \delta f_j \right) + \beta \left( \sum_{j=1}^{n_d} \frac{\partial \alpha}{\partial f_j} \Big|_{f^{\text{eq}}} \delta f_j \right) Q_i(f^{\text{eq}}). \quad (9.4)$$

Second term in (9.4) is equal to zero by the construction of the collision integral ( $Q_i(f^{\text{eq}}) = 0$ ). Denoting  $\alpha_{\text{eq}} = \alpha(f^{\text{eq}})$ , we have

$$\delta Q_i^* = \beta \alpha_{\text{eq}} \sum_{j=1}^{n_d} L_{ij} \delta f_j. \quad (9.5)$$

Linearized BGK collision integral and the single relaxation time collision integrals considered in Section 8 have the form

$$L_{ij} = -\frac{1}{\tau} (\delta_{ij} - P_{ij}), \quad (9.6)$$

where  $P_{ij}$  is the matrix of the thermodynamic projector. Only such collision integrals will be considered below.

Function  $\alpha_{\text{eq}}$  is found upon expanding Eq. (9.3) at equilibrium up to the quadratic in  $\delta f$  terms (see [1]). Using the formula for the linearized single relaxation time collision integral just derived, we find the following quadratic equation for the unknown  $\alpha_{\text{eq}}$ :

$$\frac{\alpha_{\text{eq}}^2}{2\tau^2} ((1-P)\delta f)^T * ((1-P)\delta f) - \frac{\alpha_{\text{eq}}}{\tau} (\delta f^T * ((1-P)\delta f)) = 0. \quad (9.7)$$

From the orthogonality of the thermodynamic projector it follows:

$$\delta f^T * (1-P)\delta f = (P\delta f + (1-P)\delta f)^T * (1-P)\delta f = ((1-P)\delta f)^T * (1-P)\delta f.$$

Hence, (9.7) reduces to

$$\frac{\alpha_{\text{eq}}^2}{2\tau^2} - \frac{\alpha_{\text{eq}}}{\tau} = 0, \quad (9.8)$$

and the nontrivial solution reads (see also [1]):

$$\alpha_{\text{eq}} = 2\tau. \quad (9.9)$$

Thus, the formula for the linearized dressed collision integral corresponding to a single relaxation time model (9.6) may be written in vector notation as

$$L^* = -2\beta(1-P). \quad (9.10)$$

Formulas obtained in this section will be used below when deriving the hydrodynamic limit of the discrete-time kinetic equation (9.1).

### 9.3 Multi-scale expansion

Expanding the shift operators in (9.1) to second order in  $\delta t$ , we have

$$\delta t [\partial_t + c_i \partial_x] f_i + \frac{1}{2} \delta t^2 [\partial_t + c_i \partial_x] [\partial_t + c_i \partial_x] f_i + \mathcal{O}(\delta t^3) = \beta \alpha Q_i(f). \quad (9.11)$$

Introducing a characteristic time scale  $T$  so that  $t = T t'$ , there  $t'$  is of the order 1, and also introducing  $\epsilon = \delta t / T$ , (9.11) is rewritten, omitting the error term of the order  $\epsilon^3$ ,

$$\epsilon [\partial_{t'} + c_i \partial_{x'}] f_i + \frac{1}{2} \epsilon^2 [\partial_{t'} + c_i \partial_{x'}] [\partial_{t'} + c_i \partial_{x'}] f_i = \beta \alpha Q_i(f), \quad (9.12)$$

where  $x' = (Lx)/T$  is the reduced coordinate.

Now, if  $\epsilon \ll 1$ , (9.12) is singularly perturbed (derivatives are multiplied with a small number), and thus shows a multi-scale behavior. It should be noted that the smallness parameter  $\epsilon$  is the ratio between the discretization time  $\delta t$  and the characteristic variation of the populations on a larger time and space scales,  $T$  and  $L$ , respectively. This is similar to what happens in the classical kinetic theory where the physical smallness parameter in the Boltzmann kinetic equation, Knudsen number  $\text{Kn}$ , measures the ratio between the molecular time scale (mean time of free flight of particles) relative to a characteristic time scale of hydrodynamic processes. In our case, however, there is a one more characteristic time, the discretization time  $\delta t$ . So, the origin of the multi-scale behavior is different although formally very similar to the continuous-time kinetic equations.

Solution is found in terms of the expansion,

$$f_i = f_i^{(0)} + \epsilon \delta f_i^{(1)} + \epsilon^2 \delta f_i^{(2)} + \mathcal{O}(\epsilon^3), \quad (9.13)$$

subject to the multi-scale expansion of the time derivative,

$$\epsilon \partial_{t'} = \epsilon \partial_{t'}^{(1)} + \epsilon^2 \partial_{t'}^{(2)} + \mathcal{O}(\epsilon^3). \quad (9.14)$$

Substituting (9.13) and (9.14) into (9.12), and grouping the terms of same order in  $\epsilon$ , at zeroth order we have

$$\beta \alpha (f^{(0)}) Q_i(f^{(0)}) = 0, \quad (9.15)$$

whereupon

$$f_i^{(0)} = f_i^{\text{eq}}, \quad (9.16)$$

and, taking into account the result (9.9), we also have

$$\alpha(f^{(0)}) = \alpha_{\text{eq}} = 2\tau. \quad (9.17)$$

Thus, solution in the form (9.13) concerns small deviations from the local equilibrium, as pertinent to the hydrodynamic limit,

$$f_i = f_i^{\text{eq}} + \delta f_i^{\text{neq}}. \quad (9.18)$$

The non-equilibrium part  $\delta f^{\text{neq}}$  is sought orthogonal (in the sense of the standard  $\cdot$  scalar product) to the hydrodynamic subspace. In the case of three velocities, this means

$$h_\rho^T \cdot \delta f^{\text{neq}} = 0, \quad h_u^T \cdot \delta f^{\text{neq}} = 0. \quad (9.19)$$

This orthogonality condition, as we shall see it below, immediately leads to a solvability condition which defines the unique solution  $\delta f^{\text{neq}}$ .

At first order of the multi-scale expansion we arrive at the following equation for  $f_i^{(1)}$ :

$$-2\beta \sum_{j=1}^{n_d} (1-P)_{ij} \delta f_j^{(1)} = [\partial_{t'}^{(1)} + c_i \partial_{x'}] f_i^{\text{eq}}. \quad (9.20)$$

While deriving (9.20), we have used the properties of the linearized dressed collision integral summarized in section 9.2. It is instructive to rewrite Eq. (9.20) using the geometrical language of the previous sections. To this end, we introduce the column-vector  $\Delta$  with the components

$$\Delta_i^{(1)} = (\partial_{t'}^{(1)} + c_i \partial_{x'}) f_i^{\text{eq}}. \quad (9.21)$$

With this, Eq. (9.20) reads simply

$$-2\beta(1-P)\delta f^{(1)} = \Delta^{(1)}. \quad (9.22)$$

Solvability condition (*Fredholm's alternative*) requires

$$\Delta^{(1)} \in \ker P, \quad (9.23)$$

or, in other words, that vector  $\Delta^{(1)}$  belongs to the kinetic subspace,

$$\Delta^{(1)} \in \mathcal{K}, \quad (9.24)$$

or, that it is orthogonal to the hydrodynamic subspace,

$$\mathcal{H}^T \perp \Delta^{(1)}. \quad (9.25)$$

The latter condition *defines* the action of the operator  $\partial_i^{(1)}$ . Indeed, for the basis vectors of the hydrodynamic subspace (vectors  $h_\rho$  and  $h_u$  in our case), we have

$$h_\rho^T \cdot \Delta^{(1)} = 0, \quad c h_u^T \cdot \Delta^{(1)} = 0. \quad (9.26)$$

Evaluating these scalar products, we obtain

$$\partial_{t'}^{(1)} \rho = -\partial_{x'}(\rho u), \quad \partial_{t'}^{(1)}(\rho u) = -\partial_x P^{\text{eq}}, \quad (9.27)$$

where  $P^{\text{eq}}$  is the local equilibrium pressure (see Sections 2 and 4). We remark that the definition of the action of operator  $\partial_{t'}^{(1)}$  (9.27) makes it possible to compute the first-order time derivative of any function  $\psi(\rho, \rho u)$ ,

$$\partial_{t'}^{(1)} \psi(\rho, \rho u) = \frac{\partial \psi}{\partial \rho} \partial_{t'}^{(1)} \rho + \frac{\partial \psi}{\partial(\rho u)} \partial_{t'}^{(1)}(\rho u) = -\frac{\partial \psi}{\partial \rho} \partial_x(\rho u) - \frac{\partial \psi}{\partial(\rho u)} \partial_x P^{\text{eq}}.$$

By Fredholm’s alternative, solution to (9.22) is written,

$$\delta f^{(1)} = \delta f_{\text{spec}}^{(1)} + \delta f_{\text{hom}}^{(1)}$$

where  $\delta f_{\text{hom}}^{(1)}$  is the general solution to the homogenous equation,  $(1 - P)\delta f_{\text{hom}}^{(1)} = 0$ , and  $\delta f_{\text{spec}}^{(1)}$  is a specific solution to the inhomogeneous equation (9.20). The homogeneous solution is set to zero by the orthogonality condition (9.19), while the specific solution (and hence the solution  $\delta f^{(1)}$ ) is

$$\delta f^{(1)} = -\frac{1}{2\beta} \Delta^{(1)}. \tag{9.28}$$

We remark that solution of the form (9.28) is also valid for any single relaxation time collision integral, in any dimension.

Finally, at second order of the multi-scale expansion we have:

$$\begin{aligned} & -2\beta \sum_{j=1}^{n_d} (1 - P)_{ij} \delta f_j^{(2)} - \beta \left( \sum_{k=1}^{n_d} \frac{\partial \alpha}{\partial f_k} \Big|_{f=f^{\text{eq}}} \delta f_k^{(1)} \right) \sum_{j=1}^{n_d} (1 - P)_{ij} \delta f_j^{(1)} \\ & = \partial_{t'}^{(2)} f_i^{\text{eq}} + [\partial_{t'}^{(1)} + c_i \partial_{x'}] [-\beta \sum_{j=1}^{n_d} (1 - P)_{ij} \delta f_j^{(1)} + \delta f_i^{(1)}]. \end{aligned} \tag{9.29}$$

Note that the vector of the derivatives of the function  $\alpha$  at equilibrium has to be found separately from the entropy estimate (9.3), same as it was done for the value of this function at equilibrium  $\alpha_{\text{eq}}$ . This analysis is not required here. Indeed, we are solely interested in the second-order time derivative of the locally conserved fields, and this is readily obtained from the solvability condition of (9.29). Introducing vector  $\Delta^{(2)}$  with the components

$$\Delta_i^{(2)} = \partial_{t'}^{(2)} f_i^{\text{eq}} - \frac{(1 - \beta)}{2\beta} [\partial_{t'}^{(1)} + c_i \partial_{x'}] \Delta_i^{(1)}, \tag{9.30}$$

(9.29) is written

$$-2\beta(1 - P)\delta f^{(2)} - \beta(\nabla \alpha_{\text{eq}}^T \cdot \delta f^{(1)})(1 - P)\delta f^{(1)} = \Delta^{(2)}. \tag{9.31}$$

Solvability requires

$$h_\rho^T \cdot \Delta^{(2)} = 0, \quad c h_u^T \cdot \Delta^{(2)} = 0. \tag{9.32}$$

The first condition gives

$$\partial_{t'}^{(2)} \rho = 0. \tag{9.33}$$

In other words, the first-order time derivative of the density (9.27) is exact. The second condition gives us the non-equilibrium contribution to the time derivative of the momentum,

$$\partial_{t'}^{(2)} (\rho u) = 2 \left( \frac{c_s^2 (1 - \beta)}{2\beta} \right) \partial_{x'} (\rho \partial_{x'} u). \tag{9.34}$$

While deriving the latter equation we have neglected terms of order  $u^3$  and higher (same as we did in the continuous-time derivation in Section 2). We also remind that  $c_s^2 = 1/3$ .

Finally, collecting the time derivative of the hydrodynamic fields (9.27), (9.33) and (9.34), and returning to the variables  $t$  and  $x$  we find that the entropic lattice Boltzmann scheme reconstructs the Navier-Stokes equations of the form

$$\begin{aligned} \partial_t \rho &= -\partial_x(\rho u), \\ \partial_t(\rho u) &= -\partial_x(c_s^2 \rho + \rho u^2) + 2\left(\frac{c_s^2(1-\beta)}{2\beta}\right) \partial_x(\rho \partial_x u). \end{aligned} \tag{9.35}$$

Viscosity coefficient is identified as

$$\nu = \frac{c_s^2(1-\beta)}{2\beta}. \tag{9.36}$$

Zero viscosity limit corresponds to  $\beta \rightarrow 1$ .

While the viscosity coefficient (9.36) is parameterized by  $\beta$ , where  $\beta \in [0,1)$ , it is instructive to compare it with the continuous-time result (2.23) which is parameterized by the relaxation time  $\tau$ . The relation between  $\beta$  and  $\tau$  is given by the formula (see [1] for a detailed discussion):

$$\tau = \frac{1-\beta}{2\beta}. \tag{9.37}$$

### 9.4 Example: Shock tube simulation

For a numerical illustration, we shall compare the lattice Boltzmann method for the three different collision integrals: the BGK model, the SRTM gradient-A model (8.13) and the SRTM gradient-B model (8.15). We consider evolution of a one-dimensional front in a shock tube, a very classical problem in which it appears a compressible shock front, moving into the low-density, and a rarefaction front moving into the high-density region. These two fronts leave an intermediate region in the central portion of the tube with uniform density and uniform velocity.

Runs were performed on the lattice with 800 nodes. At  $t=0$  the lattice was populated as to give the density  $\rho_- = 1.5$  for  $0 \leq x \leq 400$ , and  $\rho_+ = 1.0$  for  $400 < x \leq 800$ . Standard bounce back boundary conditions were applied at both ends of the tube. The lattice Boltzmann method (9.1) with fixed  $\alpha = \alpha_{eq}$  was used for all the three models. In Figs. 1, 2, and 3, the density profile is reported at  $t=500$  lattice time steps for the BGK, the SRTM gradient-A, and the SRTM gradient-B models, respectively. Viscosity was  $\nu = 0.06$  for all the three models, as given by the formula viscosity. As expected, in the hydrodynamic regime, all the three models are equivalent, and give practically the same result for the density.

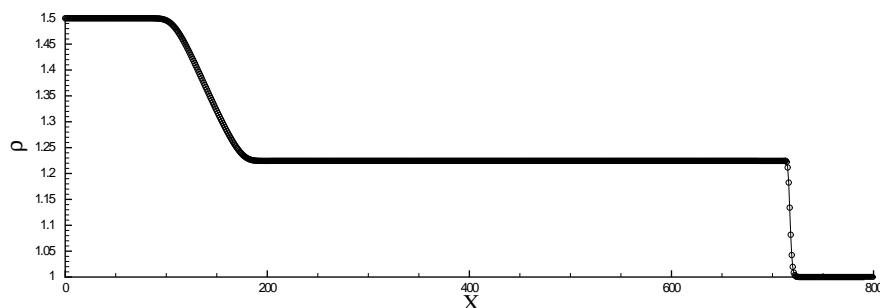


Figure 1: BGK model. Density profile in the shock tube simulation at  $t=500$ ; viscosity  $\nu=0.06$ .

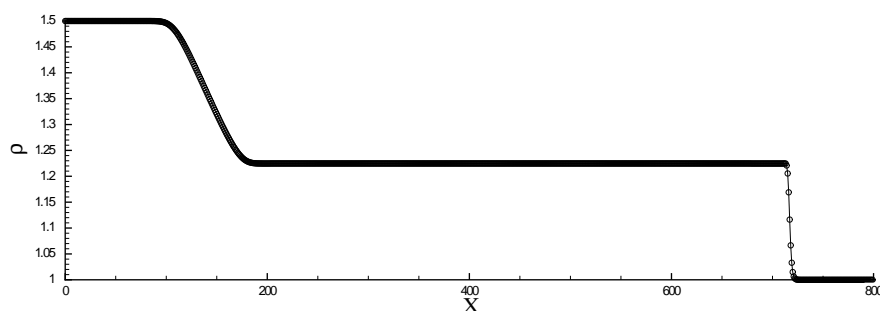


Figure 2: Gradient-A model. Density profile in the shock tube simulation at  $t=500$ ; viscosity  $\nu=0.06$ .

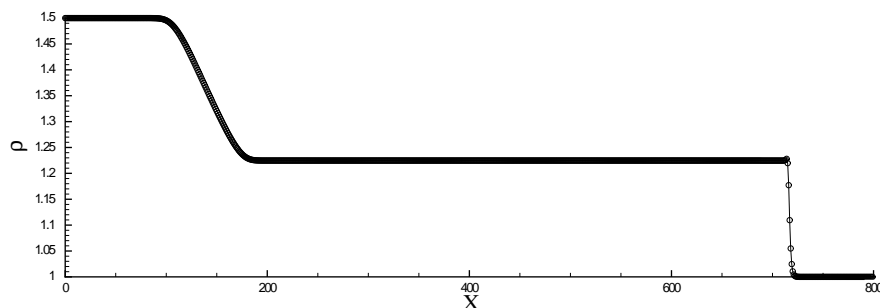


Figure 3: Gradient-B model. Density profile in the shock tube simulation at  $t=500$ ; viscosity  $\nu=0.06$ .

## 10 Conclusion

In this second paper of our series, we have considered on the example of the one-dimensional kinetic equation, the full problem of derivation of stable lattice Boltzmann schemes, beginning with the construction of the entropy function down to the entropic lattice Boltzmann scheme. We have developed a theory of admissible collision integrals and have derived new single relaxation time gradient models which are easily generalized to any dimension (some generalizations are given in the paper, and we shall consider these models in a more detail in the forthcoming contributions to this series). The next

paper will be presenting the entropic lattice Boltzmann method for three-dimensional hydrodynamics.

## A Appendix to Section 3

### A.1 General solution to (3.12)

Let us consider the *general* solution to ordinary differential equation (3.12), and find the corresponding entropy functions. Eq. (3.12) can be rewritten as  $\frac{d^2 \ln \mu_1}{d\chi^2} = 0$ , whereupon the general solution reads,  $\mu_1(\chi) = Ae^{B\chi}$ , and thus  $\mu_0(\chi) = 4Ae^{B\chi}$ . Our previous solution corresponds to  $A=e^{-1}$  and  $B=1$ . Let us carefully trace the changes caused by the general case. Inversion of the functions  $\mu_{0,1}$  reads:

$$\frac{dh_0}{d\chi} = \frac{1}{B} \ln\left(\frac{\chi}{4A}\right), \quad \frac{dh_1}{d\chi} = \frac{1}{B} \ln\left(\frac{\chi}{A}\right), \quad (\text{A.1})$$

whereupon

$$h_0(\chi) = \frac{\chi}{B} \ln\left(\frac{\chi}{4A}\right) - \frac{\chi}{B} + C_0, \quad h_1(\chi) = \frac{\chi}{B} \ln\left(\frac{\chi}{A}\right) - \frac{\chi}{B} + C_1, \quad (\text{A.2})$$

where  $C_0$  and  $C_1$  are constants (in the above derivation we have set  $C_0=C_1=0$ ). The most general form of the entropy function now follows

$$H = \frac{1}{B} \left( f_0 \ln\left(\frac{f_0}{4}\right) + f_- \ln f_- + f_+ \ln f_+ \right) - \frac{\ln A + 1}{B} \sum_{i=1}^{n_d} f_i + 2C_1 + C_0. \quad (\text{A.3})$$

The general expression (A.3) differs from (3.17) on three counts: (i) Multiplication by a positive constant  $B^{-1} > 0$ ; (ii) Adding a constant  $C = 2C_1 + C_0$ , and (iii) Adding a linear function of the density  $\rho = \sum_{i=1}^{n_d} f_i$  (multiplied by a constant  $-B^{-1}(\ln A + 1)$ ). However, *none of these differences affect the solution for the local equilibrium*. Indeed, minimization of the function (A.3) under the constraints of fixed density and momentum leads to the the following extremum conditions:

$$\begin{aligned} \frac{1}{B} \left[ \ln\left(\frac{f_0^{\text{eq}}}{4}\right) + 1 \right] - \frac{\ln A + 1}{B} &= \chi, \\ \frac{1}{B} [\ln f_{\pm}^{\text{eq}} + 1] - \frac{\ln(A) + 1}{B} &= \chi \pm \lambda v. \end{aligned} \quad (\text{A.4})$$

The Lagrange multipliers in this expression are yet undetermined, thus the factor  $B^{-1}$  and the constants can be adsorbed into the definition of the multipliers,

$$f_0^{\text{eq}} = 4 \exp(\tilde{\chi}), \quad f_{\pm}^{\text{eq}} = \exp(\tilde{\chi} \pm \tilde{\lambda} v), \quad (\text{A.5})$$



where

$$\tilde{\chi} = B \left( \chi + \frac{\ln A + 1}{B} - 1 \right), \quad \tilde{\lambda} = B\lambda. \tag{A.6}$$

The dependence of the equilibrium on the density and on the momentum is found from the constraints,  $\sum_{i=1}^{n_d} f_i^{\text{eq}} = \rho$ ,  $\sum_{i=1}^{n_d} f_i^{\text{eq}} v_i = \rho u$ , and it does not matter whether we use  $f_i^{\text{eq}}(\tilde{\chi}, \tilde{\lambda})$  or  $f_i^{\text{eq}}(\chi, \lambda)$  in the latter equations. Thus, the use of the specific  $H$  (3.17) is just *equivalent* to using any of the entropy functions (A.3).

### A.2 Derivation of the perfect entropy function from Boltzmann’s ansatz

In this Appendix we shall give an alternative derivation of the entropy function (3.17) from *Boltzmann’s ansatz* of the form

$$H = f_0 \ln \left( \frac{f_0}{W_0} \right) + f_- \ln \left( \frac{f_-}{W_1} \right) + f_+ \ln \left( \frac{f_+}{W_1} \right). \tag{A.7}$$

Our goal is to find the weights  $W_0$  and  $W_1$  such that the equilibrium pressure has the form (3.3) with the accuracy of the order  $u^4$ .

Minimization of the function (A.7) gives

$$f_0^{\text{eq}} = W_0 \exp(\chi), \quad f_-^{\text{eq}} = W_1 \exp(\chi - c\lambda), \quad f_+^{\text{eq}} = W_1 \exp(\chi + c\lambda), \tag{A.8}$$

where  $\chi$  and  $\lambda$  are Lagrange multipliers corresponding to the density and to the momentum constraints, respectively. First, we find the equilibria in a form of a velocity expansion. We expand Lagrange multipliers into powers of the velocity  $u$

$$\begin{aligned} \chi &= \chi_0 + \chi_1 u + \chi_2 u^2 + \mathcal{O}(u^3), \\ \lambda &= \lambda_0 + \lambda_1 u + \lambda_2 u^2 + \mathcal{O}(u^3). \end{aligned} \tag{A.9}$$

Substituting these expressions into (A.8), and expanding the exponentials, we obtain

$$\begin{aligned} f_0^{\text{eq}} &= W_0 e^{\chi_0} \left( 1 + \chi_1 u + \left( \frac{\chi_1^2}{2} + \chi_2 \right) u^2 \right) + \mathcal{O}(u^3), \\ f_-^{\text{eq}} &= W_1 e^{\chi_0 - c\lambda_0} \left( 1 + (\chi_1 - c\lambda_1) u + \left( \frac{\chi_1^2 + c^2 \lambda_1^2}{2} + \chi_2 - c^2 \lambda_2 \right) u^2 \right) + \mathcal{O}(u^3), \\ f_+^{\text{eq}} &= W_1 e^{\chi_0 + c\lambda_0} \left( 1 + (\chi_1 + c\lambda_1) u + \left( \frac{\chi_1^2 + c^2 \lambda_1^2}{2} + \chi_2 + c^2 \lambda_2 \right) u^2 \right) + \mathcal{O}(u^3). \end{aligned} \tag{A.10}$$

Substituting (A.10) into the constraints, and equating terms of equal orders in  $u$ , we obtain the following coefficients  $\chi_k$  and  $\lambda_k$ :

$$\begin{aligned} \chi_0 &= \ln \left( \frac{\rho}{W_0 + 2W_1} \right), \quad \chi_1 = 0, \quad \chi_2 = -\frac{W_0 + 2W_1}{4c^2 W_1}, \\ \lambda_0 &= 0, \quad \lambda_1 = \frac{W_0 + 2W_1}{2c^2 W_1}, \quad \lambda_2 = 0. \end{aligned} \tag{A.11}$$

Substituting this result into (A.10), we obtain the expansion of the equilibrium populations to second order in velocity  $u$  as a function of yet undetermined weights  $W_0$  and  $W_1$ :

$$\begin{aligned}
 f_0^{\text{eq}} &= \frac{\rho W_0}{W_0 + 2W_1} \left( 1 - \frac{u^2(W_0 + 2W_1)}{4c^2 W_1} \right) + \mathcal{O}(u^3), \\
 f_-^{\text{eq}} &= \frac{\rho W_1}{W_0 + 2W_1} \left( 1 - \frac{u(W_0 + 2W_1)}{2c W_1} + \frac{u^2 W_0(W_0 + 2W_1)}{8c^2 W_1^2} \right) + \mathcal{O}(u^3), \\
 f_+^{\text{eq}} &= \frac{\rho W_1}{W_0 + 2W_1} \left( 1 + \frac{u(W_0 + 2W_1)}{2c W_1} + \frac{u^2 W_0(W_0 + 2W_1)}{8c^2 W_1^2} \right) + \mathcal{O}(u^3).
 \end{aligned}
 \tag{A.12}$$

Note that these functions depend only on the ratio  $W_0 / W_1$ .

In the next step we compute the equilibrium pressure  $P^{\text{eq}}$ , using the expansion (A.12):

$$P^{\text{eq}} = \sum_{i=1}^{n_d} f_i^{\text{eq}} c_i^2 = c^2 f_-^{\text{eq}} + c^2 f_+^{\text{eq}} = \rho \frac{2c^2 W_1}{W_0 + 2W_1} + \rho u^2 \frac{W_0}{4W_1} + \mathcal{O}(u^4).
 \tag{A.13}$$

Note that the accuracy of the pressure (A.13) is of the fourth order in  $u$  in spite of the fact that the expansion of the equilibrium (A.12) are valid only up to the third order. Indeed, by symmetry, any terms of the order  $u^3$  cancel out in the equilibrium pressure (A.13).

We now require that the equilibrium pressure (A.13) be equal to the pressure as given by the Euler relation (3.3). That is,

$$c_s^2 = \frac{2c^2 W_1}{W_0 + 2W_1}, \quad 1 = \frac{W_0}{4W_1},
 \tag{A.14}$$

whereupon  $c_s = c / \sqrt{3}$ . Thus, we have derived the ratio of the weights (A.14) in the ansatz for the entropy function (A.7) which satisfies the pressure relation with the desired accuracy in the velocity  $u$ :

$$H = f_0 \ln \left( \frac{f_0}{4W_1} \right) + f_- \ln \left( \frac{f_-}{W_1} \right) + f_+ \ln \left( \frac{f_+}{W_1} \right).
 \tag{A.15}$$

Since adding any linear function of the locally conserved quantity (density) to the entropy function is immaterial (see previous section), we can put  $W_1 = 1$  in the latter expression to obtain again the result (3.17):

$$H = f_0 \ln \left( \frac{f_0}{4} \right) + f_- \ln f_- + f_+ \ln f_+.
 \tag{A.16}$$

The speed of sound derived herewith also coincides with the already derived value (3.11). *Comment:* This alternative derivation using a Boltzmann-like entropy function ansatz and subsequent requirements for the non-conserved moments like pressure, heat flux etc at equilibrium will be used in some derivations in the next papers of this series. However, the full derivation which does not assume any functional form of  $H$  a priori is the only systematic route to access uniqueness of the constructed entropy functions.

### A.3 Derivation of the polynomial approximation to the equilibrium

In order to derive equilibrium populations (3.18), it is sufficient to specify  $W_1 = 1$  and  $W_0 = 4$  in (A.12).

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