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Derivation of Hydrodynamics for Multi-Relaxation Time Lattice Boltzmann using the Moment Approach

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Abstract. A general analysis of the hydrodynamic limit of multi-relaxation time lattice Boltzmann models is presented. We examine multi-relaxation time BGK collision operators that are constructed similarly to those for the MRT case, however, without explicitly moving into a moment space representation. The corresponding 'moments' are derived as left eigenvectors of said collision operator in velocity space. Consequently we can, in a representation independent of the chosen base velocity set, generate the conservation equations. We find a significant degree of freedom in the choice of the collision matrix and the associated basis which leaves the collision operator invariant. We explain why MRT implementations in the literature reproduce identical hydrodynamics despite being based on different orthogonalization relations. More importantly, however, we outline a minimal set of requirements on the moment base necessary to maintain the validity of the hydrodynamic equations. This is particularly useful in the context of position and time-dependent moments such as those used in the context of peculiar velocities and some implementations of fluctuations in a lattice-Boltzmann simulation.

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1 Introduction

The lattice Boltzmann (LB) method is continuing to increase in popularity as a simulation method for fluid mechanics for a wide range of applications from turbulence [1] to complex fluids [2]. A key of its success is the simplicity of the algorithm. Instead of discretizing the hydrodynamic equations directly the method is based on an underlying microscopic model. Historically the method developed from lattice gases [3] where particles move on a lattice and collide on lattice points. Because such a lattice gas model

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locally conserves mass and momentum the macroscopic behavior of the system has to be described by the continuity and Navier-Stokes equations [4]. The connections between the microscopic streaming and collision rules and the macroscopic differential equations is established by taking the hydrodynamic limit which requires averaging the locally conserved quantities. This reproduces the Boltzmann equation [5]. Performing a Taylor expansion on the discrete Boltzmann equation then leads to a PDE representation of the discrete evolution equation [6].

At this point there are several routes to proceed. Grad [7] suggests taking moments of the full Boltzmann equation which is a route that has been taken by other groups [8]. Alternatively one can formally expand the distribution function before taking the moments, which is known as the Chapman-Enskog expansion [9]. The maximum entropy method is another viable alternative [10]. In the case of convective scaling either approach will lead to identical results to second order: the continuity and Navier-Stokes equations as well as the heat equation for thermal systems. The higher order equations are, however, quite different. Here neither approach has been particularly successful as the Navier-Stokes level equations appear to be appropriate to length-scales close to molecular scale [11]. There are few attempts to derive higher order hydrodynamic equations in the LB context. One recent publication succeeded in deriving third order hydrodynamics with an off-lattice approach [12]. Another exception are multi-phase fluids where higher order spatial derivatives giving rise to surface tension have to be taken into account [13].

The development of the method took a major leap when it was discovered that it is feasible to use a Boltzmann-level microscopic model [14, 15], which removes microscopic noise. This approach is referred to as the lattice Boltzmann method. Higuera and Jiminez already introduced the predecessor of what would become the multi-relaxation time (MRT) technique. Qian *et al.* [16] found that the approach is simplified considerably when the collision operator is written as a single-time BGK expression which relaxes local particle distributions towards the equilibrium distribution. To this date this represents the most popular flavor of lattice Boltzmann algorithms employed.

Shortly after the introduction of the single-time relaxation collision operator d'Humieres reemphasized that one can extend the BGK collision with a multi-relaxation time (MRT) approach [17]. In the MRT description the collision is described with a matrix, which allows for a decoupled relaxation of the different stress terms. It thus decouples the different transport coefficients and they no longer need to take their ideal gas values as in the single time BGK case.

Deriving hydrodynamic equations for multi-relaxation time lattice Boltzmann methods is usually achieved by Chapman-Enskog like expansions. These expansions often depend on the specific model [9]. A good review on lattice Boltzmann was published recently by Dünweg and Ladd [18]. Similar in spirit to the work presented here they attempt to derive the isothermal Navier-Stokes equations in a model independent fashion. In particular they list a set of general conditions that are required to retain hydrodynamics [Eqs. (80–84) in [18]]. However, they state that the details of the implementation of

the hydrodynamic stress cannot be done in a model independent manner. In this context we should also mention a very comprehensive approach presented by Junk *et al.* [19] detailing a very general Chapman-Enskog method for the case of diffusive scaling. In this paper we show that general requirement on the collision matrix is that it must have left eigenvectors for shear and bulk stress degrees of freedom. Furthermore we find that we are free to add any conserved quantity eigenvectors to any of the non conserved modes. Therefore we have a complete and model independent set of requirements that guarantees the validity of second order hydrodynamics. Levermore's [10] maximum entropy approach proposed a general multi-relaxation time like closure hierarchy for kinetic theories in 1996. Levermore's derivation and its application to lattice Boltzmann by Ansumali *et al.* [20] differ from the work presented here in that they do not limit themselves to the isothermal ideal gas and consequently the bulk viscosity is not a free parameter.

The relevance of this general approach stems from our interest in LB methods with locally varying collision matrices. Such an approach is necessary to address Galilean invariance in fluctuating lattice Boltzmann [21].

2 Lattice Boltzmann

The lattice Boltzmann equation (LBE) is a representation of the Boltzmann transport equation [5] with three levels discretization taken into account: time t, position $\mathbf{x}$ and velocity $\mathbf{v}$. First LB-methods utilized a two body collision operator derived from lattice gas methods (Higuera *et al.* [22]). Later Qian and D'Humieres realized that the collision operator could be significantly simplified using a BGK approach [23] as $\Omega_i = (1/\tau)(f_i^0 - f_i)$ where f_i^0 is the local equilibrium distribution [16, 17]. In the BGK approximation [23] the collision integral is replaced by a relaxation term that moves the current distribution $f(\mathbf{x},\mathbf{v},t)$ function towards the equilibrium distribution $f^0(\mathbf{x},\mathbf{v},t)$ For a general collision operator Ω_i the basic LBE can then be written as

$$f_i(\mathbf{x}+\mathbf{v}_i,t+1) - f_i(\mathbf{x},t) = \Omega_i(f_1,\cdots,f_N), \tag{2.1}$$

where the f_i are the density functions associated with a discrete set of N base velocity vectors $\mathbf{v}_i$, x is the lattice position and t is the discrete time with interval $\Delta t = 1$. The velocities are chosen such that the v_i are lattice vectors. Since collisions conserve certain quantities such as mass and momentum we require

$$\sum_i \psi_i^{a,c} \Omega_i = 0, \tag{2.2}$$

where the $\psi_i^{a,c}$ are the vectors describing the velocity moments of the conserved quantities. The index c only emphasizes that these vectors are associated with conserved quantities. We will encounter non-conserved vectors ψ^a later in this paper. The first quantity that has to be conserved in the collision is the local density which has a corresponding vector of $\psi_i^{0,c} = 1_i$ where 1_i is simply 1 for every i. Momentum must also be conserved

in each spatial direction. In three dimensions the corresponding ψ vectors are $\psi_i^{1,c} = v_{i,x}$, $\psi_i^{2,c} = v_{i,y}$, and $\psi_i^{3,c} = v_{i,z}$. We denote the locally conserved quantities as density ρ and momentum $\mathbf{j}$. They are defined through the vectors $\psi^{a,c}$ as

$$\sum_i \psi_i^{0,c} f_i = \rho, \qquad \sum_i \psi_i^{\alpha,c} f_i = j_\alpha. \tag{2.3}$$

Throughout this paper Greek indices α,β,γ will generally denote the range of spatial dimensions $\{x,y,z\}$ and be treated under the Einstein summation convention. Latin indices i,j,k are used in the context of vector components of the lattice Boltzmann base velocity set and are summed over explicitly.

Most LB models are used to simulate isothermal hydrodynamics and these models are the focus of this paper. Thermal models require the conservation of the additional moment v_i^2, which we do not treat here. In principle, however, it should be easy to extend the presented approach to thermal systems and generate the corresponding heat equation.

To recover the continuity and Navier-Stokes equations this local equilibrium distribution needs to match the first four velocity moments of the continuum Maxwell-Boltzmann distribution. This distribution is

$$f^0(\mathbf{v}) = \frac{\rho}{(2\pi\theta)^{3/2}} \exp\left(\frac{(\mathbf{v}-\mathbf{u})^2}{2\theta}\right), \tag{2.4}$$

where local velocity is defined as $\mathbf{u} = \mathbf{j}/\rho$ and θ is the temperature. For thermal models we would need to match velocity moments. The first four moments sufficient to derive isothermal hydrodynamics are

$$\sum_i f_i^0 = \rho, \tag{2.5}$$

$$\sum_i v_{i\alpha} f_i^0 = \rho u_\alpha = j_\alpha, \tag{2.6}$$

$$\sum_i v_{i\alpha} v_{i\beta} f_i^0 = \rho\theta + \rho u_\alpha u_\beta, \tag{2.7}$$

$$\sum_i v_{i\alpha} v_{i\beta} v_{i\gamma} f_i^0 = \rho\theta\left(u_\alpha\delta_{\beta\gamma} + u_\beta\delta_{\gamma\alpha} + u_\gamma\delta_{\alpha\beta}\right) + \rho u_\alpha u_\beta u_\gamma + Q_{\alpha\beta\gamma}. \tag{2.8}$$

The tensor quantity $Q_{\alpha\beta\gamma}$ is an arbitrary correction term and vanishes in the continuum case. However, the typical choice is $Q_{\alpha\beta\gamma} = -\rho u_\alpha u_\beta u_\gamma$ which allows us to use a much smaller velocity set. The trade off are small Galilean invariance problems [24]. Note that the conserved moments of the local equilibrium distribution f_i^0 and the distribution f_i are identical because the collision does not change them, *i.e.* $\sum_i \psi_i^{a,c} f_i^0 = \sum_i \psi_i^{a,c} f_i$.

Depending on the base velocity set the conditions Eqs. (2.5)-(2.8) may not uniquely define the equilibrium distribution. For practical implementations of the method we

then require a consistent choice of the f_i^0. From several different general arguments it is usually found that the explicit form

$$f_i^0(\rho,\mathbf{u}) = \rho w_i \left[(\mathbf{1} + \frac{1}{\theta}\mathbf{u}.\mathbf{v}_i + \frac{1}{2\theta^2}(\mathbf{u}.\mathbf{v}_i)^2 - \frac{1}{2\theta}\mathbf{u}.\mathbf{u} \right] \tag{2.9}$$

is a good choice for the isothermal equilibrium distribution for an appropriate choice of the w_i weight constants [25] although other forms have been used [26]. Note that we require only Eqs. (2.5)-(2.8) in the following analysis.

When deriving the hydrodynamic equations from the continuous Boltzmann equation using the single-relaxation time approximation leads to a fixed ratio of the transport coefficients such as shear viscosity, bulk viscosity, and thermal conductivity [5]. In the discrete case of lattice Boltzmann the same hydrodynamic equations can be derived with transport coefficients containing a re-normalized relaxation time $\omega = (\tau - 1/2)$. For ideal gases the predicted ratios agree quite well with the experimentally measured values [5]. The form of the hydrodynamic equations apply not only to ideal but also non-ideal gases and even fluids. Lattice Boltzmann applications usually consider examples from this more general class of systems. In these more general cases, however, the ratios of transport coefficient are no longer fixed, and it would be advantageous to write a more flexible collision term that allows for independently variable transport coefficients. This was accomplished by D'Humieres [17] by considering a multi-relaxation time BGK collision operator of the form

$$\Omega_i(f_1,\cdots,f_N) = \sum_j \Lambda_{ij}[f_j^0(\rho,\mathbf{u},\theta) - f_j(\mathbf{x},t)], \tag{2.10}$$

where Λ is a collision matrix. If we choose $\Lambda_{ij} = \delta_{ij}/\tau$ we recover the single-relaxation time collision operator. Another numerical rationale for implementing multi-relaxation time Lattice Boltzmann methods is the improvement in stability, particularly for high Reynolds numbers [27]. There are some requirements on the collision matrix to ensure mass and momentum conservation in the collision. In the single-relaxation time approach the conservation laws were respected because the conserved moments of the local distribution f_i and the local equilibrium distribution f_i^0 are identical. For the multi-relaxation time collision term Eq. (2.2) requires

$$\sum_i \psi_i^{a,c} \sum_j \Lambda_{ij} \left(f_j^0 - f_j \right) = 0. \tag{2.11}$$

These equations will be satisfied if we demand that the scalar product of a conserved quantity vector with the collision matrix is a linear combination of conserved quantity vectors, *i.e.* $\sum_i \psi_i^{a,c} \Lambda_{ij} = c^a \psi_j^{a,c}$ for an arbitrary c^a. Note here that the only physically relevant quantity is the collision operator Ω, not the collision matrix Λ. While different choices for c^a will lead to different collision matrices, they will not change the collision operator Ω. Thus Eq. (2.10) is not bijective. A convenient choice that coincides with the

single-relaxation time case sets the conserved moments 1_i and $v_{i\alpha}$ to the left-eigenvectors of our collision matrix with some eigenvalue:

$$\sum_i 1_i \Lambda_{ik} = \frac{1}{\tau_\rho} 1_k, \tag{2.12}$$

$$\sum_j v_{j\alpha} \Lambda_{ji} = \frac{1}{\tau_{j_\alpha}} v_{i\alpha}, \tag{2.13}$$

where we used the relaxation times τ to denote the inverse eigenvalues of the collision matrix. This choice also allows us to ensure that Λ is invertible which, while not strictly necessary, simplifies the formalism. Clearly, the values of $1/\tau_\rho$ and $1/\tau_{j_\alpha}$ are entirely arbitrary, meaning that τ_ρ and τ_{j_α} may not appear in the hydrodynamic equations.

3 Hydrodynamic limit by the moment method

In this section we present a new approach to obtain the hydrodynamic equations for the multi-relaxation time lattice BGK equation. We generalize the moment approach familiar from single-relaxation time methods [24] to the more general MRT formalism. For the multi-relaxation time collision operator we expand the left hand side of Eq. (2.1) to second order:

$$(\partial_t + v_{i\alpha}\partial_\alpha) f_i + \frac{1}{2}(\partial_t + v_{i\alpha}\partial_\alpha)(\partial_t + v_{i\beta}\partial_\beta) f_i + \mathcal{O}(\partial^3) = \sum_j \Lambda_{ij}\left(f_j^0 - f_j\right). \tag{3.1}$$

This allows us to write the f_i in terms of the f_i^0 and higher order derivatives as long as Λ^{-1} exists:

$$f_j = f_j^0 - \sum_i \left(\Lambda^{-1}\right)_{ji} [(\partial_t + v_{i\alpha}\partial_\alpha) f_i] + \mathcal{O}(\partial^2). \tag{3.2}$$

This is important because we can express the equilibrium distributions f_i^0 in terms of ρ and $\mathbf{u}$ in Eq. (2.9) but not the local distributions f_i. Here we have made the assumption that both, spatial and temporal derivatives, are small quantities of the same order of magnitude. As a byproduct we see that the conservation equations by virtue of Eq. (2.11) and the $\psi_i^{a,c}$ being left-eigenvectors of Λ_{ij} require

$$\sum_j \psi_j^{a,c} \sum_i \left(\Lambda^{-1}\right)_{ji} [(\partial_t + v_{i\alpha}\partial_\alpha) f_i] = \sum_i \tau^a \psi_i^{a,c} [(\partial_t + v_{i\alpha}\partial_\alpha) f_i] = \mathcal{O}(\partial^2), \tag{3.3}$$

which we will use later. Replacing all occurrences of f_i in Eq. (3.1) with Eq. (3.2) up to second order we obtain

$$\begin{aligned} &(\partial_t + v_{j\alpha}\partial_\alpha) f_j^0 - (\partial_t + v_{j\alpha}\partial_\alpha) \sum_i \left[\left(\Lambda^{-1}\right)_{ji} - \frac{1}{2}\delta_{ji}\right](\partial_t + v_{i\beta}\partial_\beta) f_i^0 + \mathcal{O}(\partial^3) \\ =& \sum_i \Lambda_{ji}\left(f_i^0 - f_i\right). \end{aligned} \tag{3.4}$$

Because we know f_i^0 as a function of ρ and $\mathbf{j}$ this is an equation expressed entirely in terms of our hydrodynamic variables, except for the collision term. So far the only requirement on the collision Matrix Λ is that it be invertible and fulfill Eq. (2.11). The general approach now to obtain a conservation equations is to take the inner product of the conserved quantity vectors $\psi^{a,c}$ with Eq. (3.4). The collision term then vanishes, we retain no dependencies on the f_i, and, after some algebra, we obtain the conservation equations.

3.1 The continuity equation

To obtain the continuity equation we take the inner product of $\psi_j^{0,c}=1_j$ with Eq. (3.4) from the left hand side, *i.e.* we just sum over Eq. (3.4) while making use of mass conservation in Eq. (2.11). We get

$$\sum_j 1_j\left(\partial_t+v_{j_\alpha}\partial_\alpha\right)f_j^0-\sum_j 1_j\left(\partial_t+v_{j\alpha}\partial_\alpha\right)\sum_i\left[\left(\Lambda^{-1}\right)_{ji}-\frac{1}{2}\delta_{ji}\right]\left(\partial_t+v_{i\beta}\partial_\beta\right)f_i^0+\mathcal{O}(\partial^3)=0. \quad (3.5)$$

We can rewrite the second order terms as

$$\partial_t\sum_j 1_j\sum_i\left[\left(\Lambda^{-1}\right)_{ji}-\frac{1}{2}\delta_{ji}\right]\left(\partial_t+v_{i\beta}\partial_\beta\right)f_i^0=\mathcal{O}(\partial^3), \quad (3.6)$$

$$\partial_\alpha\sum_j 1_j v_{j\alpha}\sum_i\left[\left(\Lambda^{-1}\right)_{ji}-\frac{1}{2}\delta_{ji}\right]\left(\partial_t+v_{i\beta}\partial_\beta\right)f_i^0=\mathcal{O}(\partial^3), \quad (3.7)$$

where we used that both 1_j and $1_j v_{j\alpha}=v_{j\alpha}$ are conserved quantity vectors so that we can apply Eq. (3.3). We are left with

$$\sum_j\left(\partial_t+v_{j_\alpha}\partial_\alpha\right)f_j^0+\mathcal{O}(\partial^3)=0, \quad (3.8)$$

which using Eq. (2.5) and Eq. (2.6) becomes the continuity equation

$$\partial_t\rho+\partial_\alpha\left(\rho u_\alpha\right)+\mathcal{O}(\partial^3)=0. \quad (3.9)$$

3.2 The Navier-Stokes equation

As the Navier Stokes equation describes the conservation of momentum we take the first order velocity moment of Eq. (3.4) and obtain

$$\sum_j v_{j\alpha}\left(\partial_t+v_{j\beta}\partial_\beta\right)f_j^0-\sum_j v_{j\alpha}\left(\partial_t+v_{j\gamma}\partial_\gamma\right)\sum_i\left[\left(\Lambda^{-1}\right)_{ji}-\frac{1}{2}\delta_{ji}\right]\left(\partial_t+v_{i\beta}\partial_\beta\right)f_i^0 +\mathcal{O}(\partial^3)=0. \quad (3.10)$$

The collision term vanishes according to Eq. (2.11). We can rewrite the first of the second order terms as

$$\partial_t \sum_j v_{j\alpha} \sum_i \left[\left(\Lambda^{-1}\right)_{ji} - \frac{1}{2}\delta_{ji} \right] \left(\partial_t + v_{i\beta}\partial_\beta\right) f_i^0 = \mathcal{O}(\partial^3), \tag{3.11}$$

which vanishes to third order due to Eq. (3.3) much like Eq. (3.7). To evaluate the remaining gradient term

$$\partial_\gamma \sum_j v_{j\alpha} v_{j\gamma} \sum_i \left[\left(\Lambda^{-1}\right)_{ji} - \frac{1}{2}\delta_{ki} \right] \left(\partial_t + v_{i\beta}\partial_\beta\right) f_i^0 \tag{3.12}$$

we need to know the stress moments $\sum_j v_{j\alpha} v_{j\gamma} \left[(\Lambda^{-1})_{ji} - \frac{1}{2}\delta_{ji} \right]$ of the collision matrix. From the single-relaxation time derivation [24] we know that these terms lead to the stress terms in the Navier-Stokes equation we wish to obtain. Because we want to distinguish between bulk and shear stress now we separate these into a trace and a traceless velocity moment

$$\sum_j v_{j\alpha} v_{j\gamma} \Lambda_{ji} = \sum_j v_{j\delta} v_{j\delta} \frac{\delta_{\alpha\gamma}}{D} \Lambda_{ji} + \sum_j \left(v_{j\alpha} v_{j\gamma} - v_{j\delta} v_{j\delta} \frac{\delta_{\alpha\gamma}}{D} \right) \Lambda_{ji}. \tag{3.13}$$

The key requirement is now that the trace and the $(D-1)\left(\frac{D}{2}+1\right)$ elements of the traceless part are left eigenvectors of the collision matrix Λ. For the trace part we demand

$$\sum_j v_{j\delta} v_{j\delta} \frac{\delta_{\alpha\gamma}}{D} \left(\Lambda^{-1}\right)_{ji} = \tau_B v_{i\delta} v_{i\delta} \frac{\delta_{\alpha\gamma}}{D}, \tag{3.14}$$

where τ_B is the bulk relaxation time and for the traceless part we require

$$\sum_j \left(v_{j\alpha} v_{j\gamma} - v_{j\delta} v_{j\delta} \frac{\delta_{\alpha\gamma}}{D} \right) \left(\Lambda^{-1}\right)_{ji} = \tau_S \left(v_{i\alpha} v_{i\gamma} - v_{i\delta} v_{i\delta} \frac{\delta_{\alpha\gamma}}{D} \right), \tag{3.15}$$

where the shear stress relaxation time τ_S is the eigenvalue. These eigenvalue equations for the second order velocity moments are the key property of the collision matrix that allows us to recover the Navier-Stokes equation. Because of the freedom to choose different eigenvalues for the trace and the traceless part we can obtain independent bulk and shear stresses.

What follows is essentially the same derivation as in the single-relaxation time case [24], except that we now have two stress terms with associated relaxation times that need to be treated independently. We use the eigenvalue equations (3.14) and (3.15) in Eq. (3.12) to replace Λ^{-1} with the appropriate eigenvalues. The different velocity moments are substituted by the expressions in Eqs. (2.5)-(2.8) and we replace $\tau_B - \frac{1}{2} = \omega_B$ and

$\tau_S - \frac{1}{2} = \omega_S$. We get

$$\begin{aligned}
&\partial_\gamma \partial_t \sum_j \sum_i v_{j\alpha} v_{j\gamma} \left[\left(\Lambda^{-1} \right)_{ji} - \frac{1}{2} \delta_{ji} \right] f_i^0 + \partial_\gamma \partial_\beta \sum_j \sum_i v_{j\alpha} v_{j\gamma} \left[\left(\Lambda^{-1} \right)_{ji} - \frac{1}{2} \delta_{ji} \right] v_{i\beta} f_i^0 \\
=& \partial_\gamma \omega_B \left[\partial_t \left(\rho u_\delta u_\delta \frac{\delta_{\alpha\gamma}}{D} + \rho\theta\delta_{\alpha\gamma} \right) + \theta \frac{D+2}{D} \delta_{\alpha\gamma} \partial_\beta \left(\rho u_\beta \right) + \frac{\delta_{\alpha\gamma}}{D} \partial_\beta \left(\rho u_\delta u_\delta u_\beta + Q_{\delta\delta\beta} \right) \right] \\
&+ \partial_\gamma \omega_S \left[\partial_t \left(\rho u_\alpha u_\gamma - \rho u_\delta u_\delta \frac{\delta_{\alpha\gamma}}{D} \right) + \partial_\beta \left(\rho\theta \left(u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\gamma\alpha} + u_\gamma \delta_{\alpha\beta} \right) + \rho u_\alpha u_\beta u_\gamma + Q_{\alpha\beta\gamma} \right) \right. \\
&\qquad \left. - \partial_\beta \left(\theta \frac{D+2}{D} \delta_{\alpha\gamma} \rho u_\beta + \frac{\delta_{\alpha\gamma}}{D} \left(\rho u_\delta u_\delta u_\beta + Q_{\delta\delta\beta} \right) \right) \right]. \qquad (3.16)
\end{aligned}$$

To treat the second order terms further we need two identities we obtain by looking at the first order terms of Eq. (3.10). Inserting the moments (2.5), (2.6) and ignoring all second order terms we get

$$\partial_t \left(\rho u_\alpha \right) = -\partial_\beta \left(\rho\theta\delta_{\alpha\beta} + \rho u_\alpha u_\beta \right) + \mathcal{O}(\partial^2). \qquad (3.17)$$

Using the continuity equation (3.9), we obtain the second identity

$$\rho \partial_t u_\alpha = -\rho u_\beta \partial_\beta u_\alpha - \partial_\beta \rho\theta\delta_{\alpha\beta} + \mathcal{O}(\partial^2). \qquad (3.18)$$

These two identities and the continuity equation (3.9) now replace the time derivatives in Eq. (3.16)

$$\begin{aligned}
&\partial_\gamma \omega_B \left\{ -\theta\delta_{\alpha\gamma} \partial_\beta \left(\rho u_\beta \right) - \frac{\delta_{\alpha\gamma}}{D} \left[u_\delta \partial_\beta \left(\rho\theta\delta_{\beta\delta} + \rho u_\beta u_\delta \right) + u_\delta \left(\rho u_\beta \partial_\beta u_\delta + \partial_\beta \rho\theta\delta_{\beta\delta} \right) \right] \right. \\
&\quad \left. + \frac{D+2}{D} \theta\delta_{\alpha\gamma} \partial_\beta \left(\rho u_\beta \right) + \frac{\delta_{\alpha\gamma}}{D} \partial_\beta \left(\rho u_\delta u_\delta u_\beta + Q_{\delta\delta\beta} \right) \right\} \\
&+ \partial_\gamma \omega_S \left\{ -u_\gamma \partial_\beta \left(\rho\theta\delta_{\alpha\beta} + \rho u_\alpha u_\beta \right) - u_\alpha \left(\rho u_\beta \partial_\beta u_\gamma + \partial_\beta \rho\theta\delta_{\gamma\beta} \right) + \partial_\beta \left(\rho u_\alpha u_\beta u_\gamma + Q_{\alpha\beta\gamma} \right) \right. \\
&\quad + \frac{\delta_{\alpha\gamma}}{D} \left[u_\delta \partial_\beta \left(\rho\theta\delta_{\beta\delta} + \rho u_\beta u_\beta \right) + u_\delta \left(\rho u_\beta \partial_\beta u_\delta + \partial_\beta \rho\theta\delta_{\beta\delta} \right) \right] + \partial_\beta \rho\theta \left(u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\gamma\alpha} + u_\gamma \delta_{\alpha\beta} \right) \\
&\quad \left. - \frac{\delta_{\alpha\gamma}}{D} \partial_\beta \left(\rho u_\delta u_\delta u_\beta + Q_{\delta\delta\beta} \right) \right\} + \mathcal{O}(\partial^3) \\
=\ & \omega_B \left[\frac{2}{D} \theta \partial_\alpha \rho \partial_\gamma u_\gamma + \frac{1}{D} \partial_\alpha \partial_\gamma Q_{\gamma\delta\delta} \right] \\
&+ \omega_S \left[\theta \partial_\gamma \left(\partial_\gamma u_\alpha + \partial_\alpha u_\gamma \right) + \partial_\beta \partial_\gamma Q_{\alpha\beta\gamma} - \frac{2}{D} \theta \partial_\alpha \rho \partial_\gamma u_\gamma - \frac{1}{D} \partial_\alpha \partial_\gamma Q_{\gamma\delta\delta} \right] + \mathcal{O}(\partial^3). \qquad (3.19)
\end{aligned}$$

If we now combine the first order terms Eq. (3.17) with the second order terms Eq. (3.19)

of the first order velocity moment of the LBE (3.10) we find the Navier-Stokes equation

$$\begin{aligned}
&\partial_t(\rho u_\alpha)+\partial_\beta(\rho u_\alpha u_\beta)\\
=&-\partial_\alpha\rho\theta+\partial_\alpha\omega_B\frac{2}{D}\theta\rho\partial_\gamma u_\gamma+\partial_\gamma\omega_S\left[\rho\theta(\partial_\gamma u_\alpha+\partial_\alpha u_\gamma)-\frac{2}{D}\theta\rho\partial_\gamma u_\gamma\delta_{\alpha\gamma}\right]\\
&+\partial_\alpha\omega_B\frac{1}{D}\partial_\gamma Q_{\gamma\delta\delta}+\partial_\gamma\omega_S\left(\partial_\beta Q_{\alpha\beta\gamma}-\partial_\gamma\frac{1}{D}Q_{\gamma\delta\delta}\right)+\mathcal{O}(\partial^3)\\
=&-\partial_\alpha\rho\theta+\partial_\alpha\mu\partial_\gamma u_\gamma+\partial_\gamma\eta[(\partial_\gamma u_\alpha+\partial_\alpha u_\gamma)-\frac{2}{D}\partial_\gamma u_\gamma\delta_{\alpha\gamma}]+\mathcal{O}(\partial^2 Q)+\mathcal{O}(\partial^3),
\end{aligned}\tag{3.20}$$

where $\mu=\frac{2}{D}\rho\theta(\tau_B-\frac{1}{2})$ is the bulk and $\eta=\rho\theta(\tau_S-\frac{1}{2})$ the shear viscosity.

In summary we recover the continuity and Navier-Stokes equations in a similar form as found from multi-relaxation time approaches with independently adjustable bulk and shear viscosities provided that three conditions are fulfilled:

1. The first four velocity moments of the equilibrium distribution are given by Eqs. (2.5)-(2.8).
2. The moments of the conserved quantity vectors 1_k and $v_{k\alpha}$ are not altered in the collision step.
3. The collision matrix has the left eigenvectors $v_{k\alpha}v_{k\beta}-v_{k\gamma}v_{k\gamma}\frac{\delta_{\alpha\beta}}{D}$ and $v_{k\gamma}v_{k\gamma}$. This has already been hinted at by Dellar in a similar context [28]. We should mention here that these left eigenvectors retain the freedom to be altered by linear combination of conserved quantity eigenvectors. This is illustrated in the next section.

Unfortunately none of the published multi-relaxation time lattice Boltzmann methods [17, 29] fulfill this last requirement. This is because we have some additional freedom in combining the ψ_i^a vectors with vectors from the conserved quantities as we will explain below. It is interesting to note that we have constraints up to the third order velocity moments for the equilibrium distribution, but only up to second order moments for the collision matrix.

We should mention that the derivation presented here does not impose any requirements on the extra degrees of freedom that are typically present in a lattice-Boltzmann implementation. A DDQQ simulation with a Q component base velocity set in D dimensions only requires $K=1+D+D(D+1)/2$ base vectors to reproduce isothermal hydrodynamics: 1 for the density, D for the momentum components, and $D(D+1)/2$ for the stress tensor. Our derivation makes no assumptions about the structure of the remaining $Q-K$ 'ghost' or kinetic modes or the choice of their corresponding relaxation times. Often the relaxation times for these ghost degrees of freedom are uniformly set to 1. In this case all possible choices for ghost eigenvectors of the collision matrix lead to identical collision matrices. The choice of ghost modes can influence the performance of the LB method if one wants to make use of the freedom to choose arbitrary relaxation times [30]. The introduction of fluctuations to the LBM requires careful treatment of the ghost modes and

their relaxation times [31], particularly in the context of boundary conditions [32]. Furthermore Adhikari and Succi suggested a duality between conserved quantity vectors and ghost modes [33] as guideline for constructing base velocity sets for multi-relaxation time implementation.

3.3 Limited freedom of choice of the eigenvectors

When we required Eqs. (3.14) and (3.15) we ignored that there is a remaining freedom of choice for the eigenvectors. To understand this, let us first remember that the relaxation times for the conserved moments τ_ρ and τ_{j_α} are entirely arbitrary by construction. Because the conserved moments of the f_i and f_i^0 are identical the collision term simply can not alter the values of the conserved quantities, independent of the value of τ_ρ and τ_{j_α}. This also implies that the effect of adding multiples of a conserved mode eigenvector $\psi_j^{a,c}$ to any of the eigenvectors will still result in suitable eigenvectors. Consider an alternative collision matrix $\hat{\Lambda}$ with a left eigenvector $\left(\psi_j^n+\psi_j^c\right)$:

$$\sum_j \left[\left(\psi_j^n+\psi_j^c\right)-\psi_j^c\right]\left(\hat{\Lambda}^{-1}\right)_{ji}=\tau^n\left(\psi_i^n+\psi_i^c\right)-\tau^c\psi_i^c. \tag{3.21}$$

Here ψ_j^n is an eigenvector of the original matrix Λ^{-1}. The n indicates that it corresponds to a non-conserved quantity and τ^n is the associated eigenvalue. In contrast ψ_j^c is an eigenvector that corresponds to a conserved quantity, i.e. ρ or v_α, with the associated eigenvalue τ^c. Now, terms that depend on τ^c have to vanish because its value is entirely arbitrary. Therefore we will only retain the $\tau^n\psi_i^n$ terms in the hydrodynamic equations. The collision matrices Λ and $\hat{\Lambda}$ will lead to identical hydrodynamic equations. To illustrate this we re-investigate the bulk stress component in the second order terms in the Navier-Stokes derivation in Eq. (3.16) for the alternative collision matrix $\hat{\Lambda}$. We replace $v_{j\delta}v_{j\delta}$ with $(v_{j\delta}v_{j\delta}+K1_j)-K1_j$ and use the aforementioned new collision matrix $\hat{\Lambda}^{-1}$ and obtain

$$\begin{aligned}
&\partial_\gamma\partial_t\sum_i\sum_j\left[(v_{j\delta}v_{j\delta}+K1_j)-K1_j\right]\left[\left(\hat{\Lambda}^{-1}\right)_{ji}-\frac{1}{2}\delta_{ji}\right]f_i^0\\
&\quad+\partial_\gamma\partial_\beta\sum_i\sum_j\left[(v_{j\delta}v_{j\delta}+K1_j)-K1_j\right]\left[\left(\hat{\Lambda}^{-1}\right)_{ji}-\frac{1}{2}\delta_{ji}\right]v_{i\beta}f_i^0\\
=&\partial_\gamma\omega_B\left[\partial_t\left(\rho u_\delta u_\delta\frac{\delta_{\alpha\gamma}}{D}+\rho\theta\delta_{\alpha\gamma}\right)+\frac{D+2}{D}\theta\delta_{\alpha\gamma}\partial_\beta\left(\rho u_\beta\right)\right]\\
&\quad-\partial_\gamma\omega_BK\left[\partial_t\rho+\partial_\beta\left(\rho u_\beta\right)\right]\frac{\delta_{\alpha\gamma}}{D}+\partial_\gamma\omega_\rho K\left[\partial_t\rho+\partial_\beta\left(\rho u_\beta\right)\right]\frac{\delta_{\alpha\gamma}}{D}.
\end{aligned}\tag{3.22}$$

For readability we omit the $\rho u_\alpha u_\beta u_\gamma+Q_{\alpha\beta\gamma}$ correction terms from Eq. (2.8) here as no additional third order velocity moments are generated by the 1_j term in the new bulk

viscosity eigenvector. The 1_j contributions lead to additional terms consisting of derivatives of the continuity equation. Since these contributions vanish to third order Eq. (3.9) the resulting Navier-Stokes equation remains unaffected. If we decided to add a first order velocity moment to one of the non-conserved eigenvectors we would find a Navier-Stokes equation instead of the continuity equation here which again vanishes to third order. We are thus free to add any vectors corresponding to our conserved quantities to the non-conserved eigenvectors. This is the degree of freedom that allows us to impose orthogonality on the eigenvectors with respect to different inner products.

To recover the approach of d'Humieres we now need to require all of the left eigenvectors of Λ_{ji} be orthogonal, with respect to the inner product $\sum_j \psi_j^m \psi_j^n = \delta_{nm} N^n$ where N^n is the norm of the vector ψ^n which need not be normalized. The only non-orthogonal left eigenvectors here are 1_j and $v_{j\gamma}v_{j\gamma}$. We remedy this by applying a Gram-Schmidt orthogonalization procedure to find the new orthogonalized bulk stress

$$v_{j\gamma}v_{j\gamma} - \frac{\sum_{j'}^{N} 1_{j'} v_{j'\gamma} v_{j'\gamma}}{N} 1_j \tag{3.23}$$

and thus recover d'Humieres' basis. In contrast recovering the Benzi approach requires that the eigenvectors obey orthogonality with respect to the Hermite norm: $\sum_j \psi_j^m \psi_j^n w_j = \delta_{mn} M^n$. Again only one pair of eigenvectors is not orthogonal, 1_j and $v_{j\gamma}v_{j\gamma}$. We apply the same orthogonalization procedure, however, with the new norm and thus obtain

$$v_{j\gamma}v_{j\gamma} - \frac{\sum_{j'}^{N} 1_{j'} w_j v_{j'\gamma} v_{j'\gamma}}{N} 1_j \tag{3.24}$$

as the orthogonal bulk stress vector. While d'Humieres' and Benzi's approaches lead to different collision matrices it is important to note that a practical implementation of the approaches is entirely identical. This is because the eigenvectors only differ by a multiple of 1_j, which is the density eigenvector and therefore a conserved quantity eigenvector.

Let us assume that we have two collision matrices Λ and $\hat{\Lambda}$ and two corresponding sets of left eigenvectors that only differ by a conserved quantity vector ψ^a and $\hat{\psi}^a = \psi^a + \psi^c$. Vectors with the same index a correspond to the same physical quantity and will thus correspond to the same time constant τ^a. The eigenvalue equations are then

$$\psi^a \Lambda = \frac{1}{\tau^a}\psi^a, \qquad (\psi^a + \psi^c)\hat{\Lambda} = \frac{1}{\tau^a}(\psi^a + \psi^c). \tag{3.25}$$

We know that conserved quantity vectors ψ^c are left eigenvectors of both Λ and $\hat{\Lambda}$ and Eq. (2.11) requires that

$$\sum_i \psi_i^c \sum_j \Lambda_{ij}\left(f_j^0 - f_j\right) = \sum_i \psi_i^c \sum_j \hat{\Lambda}_{ij}\left(f_j^0 - f_j\right) = 0, \tag{3.26}$$

independent of the actual choice of basis. Now the collision operators Ω and $\hat{\Omega}$ can be defined as

$$\Omega = \sum_j \Lambda_{ij}\left(f_j^0 - f_j\right), \qquad \hat{\Omega} = \sum_j \hat{\Lambda}_{ij}\left(f_j^0 - f_j\right). \tag{3.27}$$

Operators are defined by their action on a basis. Therefore we let Ω act on an arbitrary vector chosen from its own left eigenvector basis. Using Eqs. (3.27), (3.25), and (3.26) we get

$$\begin{aligned}\sum_i \psi_i^a \Omega_i &= \sum_i \psi_i^a \sum_j \Lambda_{ij}\left(f_j^0 - f_j\right) = \frac{1}{\tau^a}\sum_j \psi_j^a \left(f_j^0 - f_j\right) \\ &= \frac{1}{\tau^a}\sum_j \left(\psi_j^a + \psi_j^c\right)\left(f_j^0 - f_j\right) = \sum_i (\psi_i^a + \psi_i^c)\sum_j \hat{\Lambda}_{ij}\left(f_j^0 - f_j\right) \\ &= \sum_i \psi_i^a \sum_j \hat{\Lambda}_{ij}\left(f_j^0 - f_j\right) = \sum_i \psi_i^a \hat{\Omega}_i. \end{aligned} \tag{3.28}$$

Thus we have proved that as long as two different bases differ only by conserved quantity left eigenvectors, the collision operators are, in fact, identical.

4 Summary

We presented a new general formulation for the derivation of hydrodynamics. Based on the framework of generalized or multi-relaxation time formalism we performed a direct asymptotic expansion to second order of the lattice Boltzmann equation and derived the continuity and Navier-Stokes equations for the isothermal ideal gas. Our approach is general in the sense that we do not require specific knowledge of the base velocity set and equilibrium distribution function as long as the velocity moments to third order are identical to those of the continuous case and the collision does not affect the conserved quantities. We therefore do not require an explicit multi-relaxation time representation but instead describe all physically relevant quantities in terms of left eigenvectors of a collision matrix. These left eigenvectors can again be described in terms of velocity moments and thus we maintain a representation independent of the chosen base velocity set. The eigenvalues of the collision matrix are chosen to be the inverse of the relaxation time related to the physical quantity in question. Through the relaxation times associated with bulk and shear stress terms we then get direct access to the bulk and shear viscosities.

The derivation illuminates a degree of freedom in the choice of the left eigenvectors. This is rooted in the fact that the collision does not alter conserved quantities. Therefore linear combinations of conserved quantity eigenvectors can be added to non-conserved moment left eigenvectors without changing the collision operator and by extension the hydrodynamic equations. We identify this degree of freedom as the reason for the equality of multi-relaxation time implementations based on different inner products such as the standard vector and the Hermite norm. In fact, we show that for the simple case of isothermal hydrodynamics the collision operators of any two realizations of multi-relaxation time Lattice Boltzmann are identical provided they conserve mass and momentum and the appropriate equilibrium distribution is chosen.

The clear description of requirements on the collision operator and base vectors here could be particularly useful in situations where the orthogonality condition of a given

MRT implementation changes dynamically and the validity of hydrodynamics in such a case might not necessarily be obvious. One such example would be a fluctuating lattice-Boltzmann implementation where more than the zeroth order of the equilibrium distribution enter the orthogonality condition. An in-depth analysis of this case is subject of a forthcoming publication [21].

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