Galilean invariance of lattice Boltzmann models

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Abstract – It is well known that the original lattice Boltzmann (LB) equation deviates from the Navier-Stokes equations due to an unphysical velocity-dependent viscosity. This unphysical dependence violates the Galilean invariance and limits the validation domain of the LB method to near incompressible flows. As previously shown, recovery of correct transport phenomena in kinetic equations depends on the higher hydrodynamic moments. In this letter, we give specific criteria for recovery of various transport coefficients. The Galilean invariance of a general class of LB models is demonstrated via numerical experiments.

Introduction. – The idea behind the discrete-velocity kinetic method is that the full details of the single-particle distribution function in the three-dimensional microscopic velocity space is not entirely necessary in describing the thermo-hydrodynamics of a fluid. Instead, much simpler kinetic systems in which the constituent particles can only have velocities from a small discrete set can be devised to exhibit the same macroscopic behavior. This idea can be traced back to the works of Joule. It was later exploited by Broadwell [1,2] and more recently has lead to the development of the lattice gas cellular automaton (LGA) and lattice Boltzmann (LB) models [3–6]. The key question concerning the validity of this class of models is how closely the macroscopic thermo-hydrodynamics of the continuum kinetic system can be reproduced by the much simplified kinetic systems.

It is well known that the original LGA [7,8] has a non-Galilean-invariant hydrodynamics due to the artifacts in the advection term and the equation of state. The lattice BGK (LBGK) method [9,10] eliminated these artifacts by choosing a proper equilibrium distribution function in the single-relaxation-time (BGK) collision term. The Navier-Stokes hydrodynamics at the small Mach number limit is reproduced. Despite its phenomenal success in modeling near-incompressible athermal flows [11–14], the LBGK method is still not fully Galilean invariant due to a “cubic” velocity dependence of the viscosity [15], which is one of the factors that limit the valid domain of LB method to near-incompressible flows. Several attempts [16–18] have been made to overcome this short-coming using more velocities and higher-order terms in the Mach number expansion of the equilibrium distribution. The success is however limited for that not only the process of obtaining the high-order correction is tedious and model dependent, but also the Galilean invariance is in some cases only partially restored.

Recently, the LB method was re-formulated as a Hermite series solution to the continuum BGK equation [19,20], in a way similar to the Grad 13-moment system. Under this formulation, the Chapman-Enskog [21] procedure can be applied to the LBGK system in the Hermite space, revealing that the convergence of LB to continuum BGK relies on the few leading moments of the equilibrium distribution function. Provided that these moments agree with those of the Maxwell distribution, the macroscopic hydrodynamics of the LBGK equation is the same as that of the continuum BGK equation, which is known to be fully Galilean invariant. Once scrutinized in this framework, the commonly known LB models are insufficient in meeting the above conditions of retaining hydrodynamic moments, and therefore introduce errors such as the well-known cubic velocity dependence of the viscosity. This analysis is general enough so that it can be applied to the energy equation, the diffusion equation in a multi-component system, and higher hydrodynamic approximations beyond the Navier-Stokes level to give convergence criteria of other transport coefficients at the Navier-Stokes level and beyond.

In this letter, we define systematically a set of sufficient conditions for the LBGK hydrodynamics to converge to that of the continuum BGK. Essentially, these conditions are that sufficient hydrodynamic moments must be
retained in the equilibrium distribution of the LBGK system and accurately represented by the discrete velocities. We also present numerical simulation results that validate these conditions. In the next section, we first give a more elaborated derivation of the Chapman-Enskog calculation in Hermite space, and then point out the convergence condition as the direct consequence. These convergence conditions are then verified numerically by directly measuring the transport coefficients in LB simulations. Further discussions are offered in the last section.

Convergence conditions. – In a previous publication [20], the asymptotic convergence of LB to the continuum BGK was briefly shown using the Chapman-Enskog approximation procedure in Hermite space. Same as in continuum kinetic theory, the macroscopic equations of LB are essentially determined by the leading tensorial hydrodynamic moments. With discrete velocities, these moments are expressed as weighted sum of tensors constructed from discrete velocities, which are not always isotropic as their continuum counterparts are. The insufficient isotropy of certain moments has long been recognized as one of the reasons responsible for the deviations from the continuum hydrodynamics. By expanding the distribution function in Hermite polynomials, this tedious calculation can be tremendously simplified and extended to higher orders.

We first note that the hydrodynamic equations are given by the conservations of mass, momentum and energy. Omitting external forces, they are:

\[
\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{u} = 0,  \tag{1}
\]

\[
\frac{d\mathbf{u}}{dt} + \nabla \cdot \mathbf{P} = 0,  \tag{2}
\]

\[
\frac{d\epsilon}{dt} + \mathbf{P} \cdot \nabla \mathbf{u} + \frac{1}{2} \nabla \cdot \mathbf{S} = 0,  \tag{3}
\]

where \(d/dt\) represents the substantial derivative and the density \(\rho\), the fluid velocity \(\mathbf{u}\), the internal energy density \(\epsilon\), the pressure tensor \(\mathbf{P}\) and the heat flux \(\mathbf{S}\) are all velocity moments of \(f\):

\[
\rho = \int f \, d\xi, \tag{4}
\]

\[
\rho \mathbf{u} = \int f \mathbf{u} d\xi, \tag{5}
\]

\[
\rho \epsilon = \frac{1}{2} \int f \vert \mathbf{u} \vert^2 \, d\xi, \tag{6}
\]

\[
\mathbf{P} = \int f (\xi - \mathbf{u}) (\xi - \mathbf{u}) d\xi, \tag{7}
\]

\[
\mathbf{S} = \int f \vert \mathbf{u} \vert^2 (\xi - \mathbf{u}) d\xi, \tag{8}
\]

where \(f\) is the single-particle distribution function and \(\xi\) the microscopic velocity. Clearly, two distribution functions with the same leading velocity moments will yield the same hydrodynamic equations.

For closing eqs. (1)–(3), the task of obtaining the approximated distribution function using the few hydrodynamic moments was in the center of the development of the kinetic theory in the last century. In the Chapman-Enskog calculation, a successive sequence of approximated distribution functions are introduced in the order of Knudsen number [21]. For the following Boltzmann equation with the BGK collision model [22]:

\[
\frac{\partial f}{\partial t} + \xi \cdot \nabla f = -\frac{1}{\tau} [f - f^{(0)}], \tag{9}
\]

where \(\tau\) is the relaxation time, the \(i\)-th approximation of the distribution is given by the recursive relation:

\[
f^{(i)} = -\tau \left( \frac{\partial}{\partial t} + \xi \cdot \nabla \right) f^{(i-1)}, \quad i = 1, 2, \ldots, \tag{10}
\]

with \(f^{(0)}\) the Maxwell-Boltzmann distribution. On substituting \(f^{(i)}\) into eqs. (1)–(3) for \(i = 0, 1, 2\) and using results of the previous approximation, the hydrodynamic equations at the Euler, the Navier-Stokes, and the Burnett levels are obtained [23]. This sequence of approximation quickly becomes formidably complex beyond the first two.

Equation (10) implies a simple recursive relation among the moments of the distribution functions at various approximation levels. We note that the velocity moments of the distribution function are essentially its Hermite coefficients [24]. Let \(a^{(n)}_i\) be the \(n\)-th Hermite coefficient of the distribution \(f^{(i)}\). As previously shown, on substituting the corresponding Hermite expansions into eq. (10), the Hermite coefficients of the first approximation can be explicitly expressed using the Hermite coefficients of the zero-th approximation, namely:

\[
a^{(n)}_1 = -\tau \left[ \frac{\partial a^{(n)}_0}{\partial t} + \nabla a^{(n-1)}_0 + \nabla \cdot a^{(n+1)}_0 \right]. \tag{11}
\]

From the above equation, an important conclusion that can be immediately drawn about the BGK equation (9) is that the leading \(n\) moments in the first approximation, which gives the Navier-Stokes hydrodynamics, is given by the leading \(n + 1\) moments of \(f^{(0)}\). The form of the hydrodynamic equations is completely determined by the few leading moments of \(f^{(0)}\). For instance, at the Navier-Stokes level \((i = 1)\), \(\mathbf{P}\) is determined by \(a^{(2)}_1\), which is in turn determined by the expansion coefficients of \(f^{(0)}\) up to \(a^{(3)}_0\). Therefore, the momentum equation is correct as long as \(f^{(0)}\) agrees with the Maxwellian in the first three terms of their Hermite expansions.

For a finite sum of Hermite series, the leading moments are completely determined by the function values at a finite set of abscissas. This property, together with the fact that the hydrodynamic equations are determined by the finite number of leading Hermite terms of \(f^{(0)}\), allows a discrete-velocity kinetic system to have the same macroscopic hydrodynamics as the continuum system.
when their leading moments are the same. Consider a finite sum of Hermite series as \( f^{(0)} \):

\[
f^{(0)} = \omega(\xi) \sum_{i=0}^{N} \frac{1}{n!} a^{(n)}_{0} H^{(n)}(\xi).
\]

Let \( M \) be the highest order of the moments that determines the hydrodynamic equations of interest, e.g., \( M = 3 \) if the momentum equation at the Navier-Stokes level is of concern. The leading \( M (\leq N) \) moments are in the form of

\[
\int \omega(\xi) p(\xi) d\xi,
\]

where \( p(\xi) \) is a polynomial of an order \( \leq M + N \). This integral can be exactly evaluated using the values of the integrand on a finite set of velocities, \( \{ \xi_{i} : i = 1, \ldots, d \} \), as

\[
\int \omega(\xi) p(\xi) d\xi = \sum_{i=1}^{d} w_{i} p(\xi_{i}),
\]

if and only if \( \xi_{i} \) are the abscissas of a Gauss-Hermite quadrature of a degree of precision \( Q \geq M + N \), and \( w_{i} \) the corresponding weights. It can now be concluded that the sufficient conditions for the LBGK system to have the correct hydrodynamic equations are:

1) The equilibrium distribution retains the necessary moments.

2) The discrete velocity set allows the moments to be exactly evaluated using finite function values.

Quantitatively, these two conditions are:

\[
N \geq M \quad \text{and} \quad M + N \leq Q.
\]

Since \( Q \) is finite for any finite set of velocities and \( N \leq Q \), \( N \) must be finite, i.e., the equilibrium distribution in LBGK is the sum of a finite Hermite series of an order which is smaller than the degree of the quadrature. The difference between \( Q \) and \( N \) is the maximum order of the moments whose dynamics will be the same as that in the continuum system.

The requirements for the momentum equation to be fully Galilean invariant at the Navier-Stokes level are immediately clear. Since \( M = 3 \) in this case, we have \( N \geq 3 \) and \( Q \geq 6 \). Namely \( f^{(0)} \) must retain all Hermite terms up to the third order and the discrete velocity set must form a 6th-order accurate Hermite quadrature. Neither of the original LBGK models [9,10] satisfies this condition as only the second-order terms are retained and the velocity set is only 5-th order in both cases (\( Q = 5 \)). As the velocity set is sufficient to support the second-order terms, the error introduced in both models are due to the last term on the right-hand side of eq. (11), which manifests as the “cubic” velocity dependence of the viscosity [15,20].

The analysis above can be applied to the case of energy equation where full recovery of the Navier-Stokes energy equation requires \( N \geq M \geq 4 \), and \( Q \geq 8 \). Using a third-order expansion (\( N = 3 \)), or a velocity set that only supports third-order moments (\( 6 \leq Q < 8 \)) could yield otherwise correct thermal LBGK models with a velocity-dependent thermal diffusivity.

It is worth pointing out that when conditions (15) are satisfied, the equilibrium function of eq. (12) results in the exact hydrodynamics equations regardless of the Mach number. Hydrodynamic moments up to a given order can be shown to have the same dynamics of their continuum counterparts. These conditions are also necessary if a finite-order polynomial is used as the the equilibrium distribution. Nevertheless, it was shown previously [25,26] that discrete velocity models can be constructed with exact conservation laws and correct higher moments in the small Mach number limit.

We note that for a given set of velocities and weights, \( Q = \{ (\xi_{i}, w_{i}) : i = 1, \ldots, d \} \), the isotropy of the following tensors play a critical role in the analysis of LGA and LBGK [8].

\[
E^{(n)} = \sum_{i=1}^{d} w_{i} \prod_{n \text{ times}} \xi_{i}.
\]

Here, we point out that \( Q \) corresponding to a \( Q \)-th order Gauss-Hermite quadrature is equivalent to the condition that:

\[
E^{(n)} = \begin{cases} 0, & n \text{ odd}, \\ \delta^{(n)}, & n \text{ even}, \end{cases} \forall n \leq Q,
\]

where \( \delta^{(n)} \) is the rank-\( n \) isotropic tensor. Noticing that the above is always true in continuum, i.e., after defining \( p^{(n)}(\xi) \equiv \prod_{n \text{ times}} \xi_{i} \), we have:

\[
\int \omega(\xi) p^{(n)}(\xi) d\xi = \begin{cases} 0, & n \text{ odd}, \\ \delta^{(n)}, & n \text{ even}, \end{cases}
\]

the forward equivalence is trivial since \( \forall n \leq Q \), \( p^{(n)}(\xi) \) is a polynomial of a degree \( \leq Q \). Because of eq. (14),

\[
E^{(n)} = \int \omega(\xi) p^{(n)}(\xi) d\xi = \begin{cases} 0, & n \text{ odd}, \\ \delta^{(n)}, & n \text{ even}. \end{cases}
\]

The backward equivalence is also straightforward. As \( \{ p^{(n)}(\xi) : n \leq Q \} \) is a linearly independent set and forms a complete basis of the Hilbert space of all polynomials of a degree \( \leq Q \), any such polynomial can be written as a linear combination of \( p^{(n)}(\xi) \). By direct integration, it can be shown that eq. (14) is true as long as eq. (17) is true. Condition (17) is also proved by a slightly different procedure elsewhere [27].

**Numerical simulations.** To numerically demonstrate the theory outlined in the previous section, here we present simulation results of some simple benchmarking problems using LBGK models with equilibrium distributions and velocity sets of different orders. All
Table 1: The abscissas and weights of a ninth-order accurate Gauss-Hermite quadrature formula in three dimensions. Here \( p \) is the number of abscissas in the symmetry class. The subscript \( FS \) denotes a fully symmetric set of points.

| \( \xi \)         | \( p \) | \( w_n \) |
|-------------------|--------|----------|
| \((0, 0, 0)\)     | 1      | 0.0305916220984860642469 |
| \((r, 0, 0)_{FS} \) | 6      | 0.098515951037236339186467 |
| \((\pm r, \pm r, r)\) | 8      | 0.0275250532563812386479 |
| \((r, 2r, 0)_{FS} \) | 24     | 0.0061110233636834232241 |
| \((2r, 2r, 0)_{FS} \) | 12     | 0.004281835936810406618 |
| \((3r, 0, 0)_{FS} \) | 6      | 0.00324747570807381296 |
| \((2r, 3r, 0)_{FS} \) | 24     | 0.0001431862411548029405 |
| \((\pm 2r, \pm 2r, \pm 2r)\) | 8      | 0.0001810217515763743759 |
| \((r, 3r, 0)_{FS} \) | 24     | 0.00010683400245939109491 |
| \((\pm 3r, \pm 3r, \pm 3r)\) | 8      | 0.00000069287508963860285 |

Fig. 1: Velocity dependence of viscosity of the fifth-order D3Q19 model (top) and the seventh order 39-velocity model (bottom) using second- and third-order equilibrium distribution function. Here, \( \nu_0 \) is the theoretical value of viscosity at zero mean velocity and \( c = \sqrt{T_0} \) is the isothermal sound speed.

The viscosity is measured through the decay rate of the amplitude. Shown in Fig. 1 are the measured viscosity, normalized with respect to its theoretical value, as a function of the longitudinal and transverse components of \( u_0 \). Here the magnitude of \( u_0 \) are expressed in terms of the corresponding Mach numbers. On the top are the results using the 19 point (D3Q19) model with second- and third-order equilibrium distribution function (\( N = 2 \) and 3, respectively). The dependence, on the translational velocity is significant in both cases except for small Mach numbers. For the case of \( N = 2 \), the error is caused by the missing third-order term in the equilibrium distribution function. For the case of \( N = 3 \), the 19-velocity quadrature is not sufficiently accurate for the third-order moments and results in an error in another form. On the bottom are results using the 39-velocity model. To be seen is that the velocity dependence of the viscosity is removed once the third-order term is included in the equilibrium distribution function.

The thermal diffusivity is measured in a similar fashion. Instead of velocity, an initial sinusoidal temperature perturbation is imposed while both the velocity and pressure are uniform. Figure 2 shows the thermal diffusivity as a function of the translational velocity \( u_0 \) and the background temperature \( T_0 \). Here \( u_0 \) is taken to have the
equal components in three directions. As shown in fig. 2a, with the third-order equilibrium distribution function, the diffusivity varies with the translational velocity. Furthermore, this dependence of the velocity also depends on the background temperature. As shown in fig. 2b, when the fourth-order equilibrium distribution function is used, the thermal diffusivity does not depend on the translational velocity anymore and agrees well with the theoretical value for different background temperatures. The Galilean invariance is completely recovered. However, the stability of the model depends on the background temperature and translational velocity. Hence, in fig. 2, there are no data for some high-velocity cases. A detailed discussion of the instability is beyond the scope of this paper.

**Discussion.** – In this letter, we give the quantitative conditions for the LBGK system to have the same macroscopic hydrodynamics as the continuum kinetic system described by the BGK equation. The degree of precision of the velocity set as a Gauss-Hermite quadrature together with the order of the Hermite terms retained in the distribution function determines the order of the hydrodynamic moments that will have the correct macroscopic behavior. The velocity dependence of the viscosity in the commonly used LBGK system is identified as an error due to both the insufficient truncation of the distribution function in moment space and the insufficient isotropy of the 9-velocity model. Once sufficient moments are retained in the equilibrium distribution and accurate quadrature is used, the hydrodynamic behavior of the LBGK asymptotically approaches to that of the BGK equation in continuum. Kinetic models for thermal fluids, fluid mixtures and fluids beyond Navier-Stokes hydrodynamics can be constructed with guaranteed Galilean invariance.

Centered in the effort of restoring full Galilean invariance in the LBGK system is the search for a velocity set that makes isotropic tensors. This effort is shown here to be equivalent to finding the sufficiently accurate Hermite quadratures. On a regular Cartesian grid, this task was solved systematically [20, 29]. To fully recover the Galilean invariant Navier-Stokes momentum equation, sixth-order accurate quadratures are required. It can be verified that with the D2Q17 model [17], the diagonal component of the sixth tensor is not isotropic, causing the Galilean invariance not fully restored in the corresponding terms. Through exhaustive search, it can be concluded that to have the sixth-order isotropy with velocities forming a regular lattice, speed-3 velocities must be included. The minimum velocity set found on a regular grid with sixth-order isotropy is the 39-velocity model in three dimensions and the 21-velocity model in two dimensions. A different velocity set with a sixth-order isotropy has been given by Chikatamarla et al. [26]. However, smaller velocity sets not entirely on a regular grid are also available [20].

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