Vol 18 No 6, June 2009
1674-1056/2009/18(06)/2159-09

Chinese Physics B

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Thermal equation of state for lattice Boltzmann gases*

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(Received 23 July 2008; revised manuscript received 1 December 2008)

The Galilean invariance and the induced thermo-hydrodynamics of the lattice Boltzmann Bhatnagar–Gross–Krook model are proposed together with their rigorous theoretical background. From the viewpoint of group invariance, recovering the Galilean invariance for the isothermal lattice Boltzmann Bhatnagar–Gross–Krook equation (LBGKE) induces a new natural thermal-dynamical system, which is compatible with the elementary statistical thermodynamics.

Keywords: lattice Boltzmann method, thermal equation of state, Galilean invariance
PACC: 0500, 0520, 0520D, 0570C

1. Introduction

The lattice Boltzmann method (LBM) is a powerful new approach to hydrodynamics, with applications ranging from large Reynolds number flows in microscale porous media to multiphase flows.[1−4] In spite of a large number of studies that have been carried out to date, there are still several directions where the lattice Boltzmann theory calls for substantial progress and upgrades. For example, the correct treatment of energy degrees of freedom in a lattice still poses a number of basic questions. Furthermore, full thermohydrodynamic LBM schemes represent a standing challenge to the LBM research.[5] It is also noted that another important problem related to the LBM, recognized by many authors, is the problem of Galilean invariance.[6−9] The present paper will be devoted to the invariance problem of the lattice Boltzmann equation, including the induced thermodynamics of the LBM based on the well developed Lie group analysis skills. It is hoped that the Lie symmetry analysis will throw some light upon this subject.

Symmetry has always played an important role in mechanics, from fundamental formulations of basic principles to concrete applications.[10−12] Applications of symmetry groups to numerical analysis are given an extensive treatment in Refs.[13] and [14]. For gas dynamics, Yanenko and Shokin[15] used the first differential approximation to make a group analysis. The symmetries of difference equations were studied much more early than differential equations. Early work in this direction was done by Maeda.[16] He studied only transformations acting on the dependent variables. More recently a series of papers was devoted to Lie point symmetries of differential difference equations, which can be found in Refs.[17]–[19]. The overall theme is called "continuous symmetries of discrete equations". As is well known, the dynamics of most physical processes is described by differential equations. Lie group theory provides a powerful tool for obtaining exact analytical solutions of such equations, specially the most fundamental ones that are usually nonlinear (the Einstein equations, the Yang–Mills equations, the Navier–Stokes equations, ...). In many cases, the symmetries of differential equations are more important and better known than the equations themselves since these symmetries reflect fundamental physical laws. Thus, when we use the LBM, otherwise modifying the dynamical equations, it is of interest to preserve the original symmetries.

The remainder of the present paper is organized as follows. A briefing of the theory of symmetries of differential equations is given in Section 2. Section 3 is devoted to the group calculation of the one-dimensional gas dynamics and a complete development of the application to the invariance of LBM: two special cases of interest. Finally the conclusions drawn from the present study are presented in Section 4.

*Project supported by the National Natural Science Foundation of China (Grant Nos 90816013 and 10572083), and Shanghai Leading Academic Discipline Project, China (Grant No Y0103).

2. Invariance of lattice Bhatager–Gross–Krook (LBGK) model

2.1. Symmetries of differential equations

All the problems that we will address here may be described by a general system of n-th order nonlinear differential equations

$$\Delta_\nu \left(x, u^{(n)}\right) = 0, \tag{1}$$

where $\nu = 1, \dots, l$, $x = \left(x^1, \dots, x^p\right) \in X$ are independent variables, $u = \left(u^1, \dots, u^q\right) \in U$ are dependent variables and $\Delta_\nu \left(x, u^{(n)}\right) = \left(\Delta_1 \left(x, u^{(n)}\right), \dots, \Delta_l \left(x, u^{(n)}\right)\right)$ is a smooth function depending on x, u and the first, second, $\dots$, n-th derivatives of u with respect to $x^1, \dots, x^p$. If we define a jet space $X \times U^{(n)}$ as a space whose coordinates are independent variables, dependent variables and the first, second, $\dots$, n-th derivatives of dependent variable U then Δ is a smooth mapping

$$\Delta : X \times U^{(n)} \to R^l. \tag{2}$$

Before studying the symmetries of difference schemes, we briefly review the theory of the symmetries of differential equations. For all details, proofs and further information we have referred to some excellent books on the subject, e.g. Refs.[10] and [11]. Here, we follow the style of Ref.[10], but just give a briefing of the Lie symmetry by emphasizing the important points and significant results. In order to provide readers with a relatively quick and painless introduction to the Lie symmetry theory, some important concepts must be introduced.

The main tool in the theory of Lie groups and transformation groups is the "infinitesimal transformation". In order to present this, we need first to develop the concept of a vector field on a manifold. We begin with a discussion about tangent vectors. Suppose that C is a smooth curve on manifold M, parameterized by

$$\phi : I \to M, \tag{3}$$

where I is a subinterval of R. In local coordinates $x = \left(x^1, \dots, x^p\right)$, C is given by p smooth functions

$$\phi(\varepsilon) = \left(\phi^1(\varepsilon), \dots, \phi^p(\varepsilon)\right) \tag{4}$$

of real variable ε. At point $x = \phi(\varepsilon)$ of C the curve has a tangent vector, namely the derivative

$$\dot{\phi} = \frac{\mathrm{d}\phi}{\mathrm{d}\varepsilon} = \left(\frac{\mathrm{d}\phi^1}{\mathrm{d}\varepsilon}, \dots, \frac{\mathrm{d}\phi^p}{\mathrm{d}\varepsilon}\right). \tag{5}$$

In order to distinguish between tangent vectors and local coordinate expressions for a point on the manifold, we adopt the notation

$$V = \frac{\mathrm{d}\phi}{\mathrm{d}\varepsilon} = \frac{\mathrm{d}\phi^1}{\mathrm{d}\varepsilon} \cdot \frac{\partial}{\partial x^1} + \cdots + \frac{\mathrm{d}\phi^p}{\mathrm{d}\varepsilon} \cdot \frac{\partial}{\partial x^p} \tag{6}$$

for the tangent vector to C at $x = \phi(\varepsilon)$. The collection of all tangent vectors to all possible curves passing through a given point x in M is called the tangent space to M at x and denoted by TM. A vector field V on M assigns a tangent vector $V \in TM$ to point $x \in M$, with V varying smoothly from point to point. In local coordinates, a vector field has the form

$$V = \xi^1(x) \cdot \frac{\partial}{\partial x^1} + \cdots + \xi^p(x) \cdot \frac{\partial}{\partial x^p}, \tag{7}$$

where $\xi^i(x)$ is a smooth function of x.

If V is a vector field, we denote the parameterized maximal integral curve passing through x in M by $\Psi(\varepsilon, x)$ and call Ψ the flow generated by V. Thus for point x in M, and ε in some interval I_x containing 0, $\Psi(\varepsilon, x)$ will be a point on the integral curve passing through x in M. The flow of a vector field has the basic properties

$$\Psi(\delta, \Psi(\varepsilon, x)) = \Psi(\delta + \varepsilon, x), \tag{8}$$

for all $\delta, \varepsilon \in R$ such that both sides of equation are defined,

$$\Psi(0, x) = x, \tag{9}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon} \Psi(\varepsilon, x) = V \tag{10}$$

for all values of ε in the region where they are defined. The flow generated by a vector field is the same as a local group action of the Lie group on the manifold M, which is often called the one-parameter group of transformations. The vector field V is called an infinitesimal generator of the action since by Taylor's theorem, in local coordinates

$$\Psi(\varepsilon, x) = x + \varepsilon \xi(x) + O\left(\varepsilon^2\right), \tag{11}$$

where $\xi = \left(\xi^1, \dots, \xi^p\right)$ are the coefficients of V. The orbits of the one-parameter group action are the maximal integral curves of the vector field V.

Definition 1 A symmetry group of Eq.(1) is the one-parameter group of transformations, G, acting on $X \times U$ such that if $u = f(x)$ is an arbitrary solution

of Eq.(1) and $g_\varepsilon \in G$ then $g_\varepsilon \cdot f(x)$ is also a solution of Eq.(1).

The infinitesimal generator of a symmetry group is called an infinitesimal symmetry. To formulate the condition for group G to become a symmetry group we use infinitesimal generators. It is easy to obtain infinitesimal generators. First we define a prolongation of a vector field. The symmetry group of a system of differential equations is the largest local group of transformations acting on the independent and dependent variables of the system with the property that it transforms solutions of the system into other solutions. The main goal of the Lie symmetry theory is to present a useful systematic computational method, which can be used to explicitly determine the symmetry group of any given system of differential equations. The search for the symmetry algebra L of a system of differential equations is best formulated in terms of vector fields acting on the space $X \times U$ of independent and dependent variables. The vector field tells us how the variables x and u are transformed. We also need to know how the derivatives like $u_x,\ u_{xx}, \dots$ are transformed. These can be given by the prolongation of the vector field V. We have the following theorems. (see Theorem 2.36, p.110, in Ref.[10])

Theorem 1. Let

$$V = \sum_{i=1}^{p} \xi^i (x,u)\, \partial_{x^i} + \sum_{a=1}^{q} \eta_a (x,u)\, \partial_{u^a}$$

be a vector defined on an open subset $M \subset X \times U$. The n-th prolongation of the vector field is the vector field

$$pr^{(n)} V = V + \sum_{a=1}^{q} \sum_{J} \eta_a^J \left(x, u^{(n)}\right) \frac{\partial}{\partial u_J^a},$$

defined in the corresponding jet space $M^{(n)} \subset X \times U^{(n)}$, where the second summation is performed over all (unordered) multi-indices $J = (j_1, j_2, \dots, j_k)$, with $1 \le j_k \le p$, $1 \le k \le n$. The coefficient function ϕ_a^J of $pr^{(n)} V$ is given by the following formula:

$$\eta_a^J \left(x, u^{(n)}\right) = D_J \left(\eta_a - \sum_{i=1}^{p} \xi^i u_i^a\right) + \sum_{i=1}^{p} \xi^i u_{J,i}^a,$$

where $u_i^a = \partial u^a / \partial x^i$, $u_{J,i}^a = \partial u_J^a / \partial x^i$, and D_J is the total derivative of η with respect to x^j.

In the following analysis, we deal only with the one-dimensional scalar differential equations, and the functions treated in this paper are assumed to be differentiable up to a necessary order. In the future analysis of the difference equation, we will deal with the modified equation, which has the third prolongation of the vector field. From the computational fluid dynamics (CFD), we know that the terms on the right-hand side of the modified equation are written entirely in terms of derivative with respect to x. So we can consider only the terms of the spatial derivatives in the following analysis. It is assumed that an n-th-order system of differential equations, or, equivalently, a subvariety of the jet space $M^{(n)} \subset X \times U^{(n)}$ is given. A symmetry group of this system is defined as local transformation G acting on $M \subset X \times U$ which transforms solutions of the system into other solutions. We can deduce the important infinitesimal condition for group G to become a symmetry group of a given system of differential equations. The following theorem (see Theorem 2.31, p.104, Ref.[10]) gives infinitesimal condition for group G to become a symmetry group.

Theorem 2 Suppose that

$$\Delta_\nu \left(x, u^{(n)}\right) = 0,\ \nu = 1, 2, \dots, l,$$

is a system of differential equations of maximal rank defined over $M \subset X \times U$. If G is a local group of transformation acting on M, and

$$pr^{(n)} V \left[\Delta_\nu \left(x, u^{(n)}\right)\right] = 0,\ \nu = 1, 2, \dots, l,$$

when $\Delta_\nu \left(x, u^{(n)}\right) = 0$ for infinitesimal generator V of G, then G is a symmetry group of the system.

In the following sections, we will use this theorem to deduce explicitly the different infinitesimal conditions for relevant problems. But we must keep in mind that in all cases, though we deal only with the scalar differential problem, we still use Δ_ν to denote different differential equations.

Theorem 1 tells us how to obtain an explicit expression of prolongation of the group, while theorem 2 provides us with an explicit expression of the invariance. These theorems form the basis of our further research. It should be pointed out that in the future analysis of the difference equation, we will deal with the modified equation, which has the second/third order prolongation of the vector field. From the computational fluid dynamics (CFD), we know that the terms on the right-hand side of the modified equation are written entirely in terms of spatial derivatives. So we can consider only the terms of the spatial derivatives in the following analysis.

2.2. Invariance of one-dimensional gas dynamics

Now we come to consider a system of equations of gas dynamics in Eulerian coordinates in the case of one space variable, given as

$$\frac{\partial W}{\partial t}+\frac{\partial F}{\partial x}=0, \tag{12}$$

where

$$W=\begin{bmatrix}\rho\\ \rho u\\ \rho E\end{bmatrix},$$

$$F=\begin{bmatrix}\rho u\\ p+\rho u^2\\ up+\rho uE\end{bmatrix},$$

and

$$E=e+\frac{1}{2}u^2,$$

u is the gas speed, p is the pressure, ρ is the density, e is the specific internal energy. The equation of state of gas has the form

$$e=e\left(p,\rho\right). \tag{13}$$

It is well known that the system of one-dimensional gas equations admits a space of operators with the basis

$$V_1=\partial_t, \tag{14}$$

$$V_2=\partial_x, \tag{15}$$

$$V_3=t\partial_x+\partial_u, \tag{16}$$

$$V_4=x\partial_x+t\partial_t, \tag{17}$$

which represent, respectively, the following finite transformations with preserving the system of equations:

(i) translation in time; (ii) translation in a space coordinate; (iii) Galilean transformation; (v) similarity transformation.

2.3. Galilean invariance of one-dimensional LBM

The classical Chapman–Enskog expansions provide a natural bridge between the kinetic description of gas dynamics as given by the Boltzmann equation and that of continuum mechanics as given by the balance laws of mass, momentum, energy supplemented. To start with, we present the detailed analysis on a typical one-dimensional lattice Boltzmann equation (LBE) the 1D3Px model.[3] In 1992, Qian *et al*[4] proposed the LBGK model as an alternative to lattice gases or the LBE, to obtain an efficient numerical scheme for the simulation of fluid dynamics. With an appropriately chosen equilibrium distribution, the Navier–Stokes equation is obtained from the kinetic BGK equation in the second-order of approximation. The main idea could be presented as follows.

The requirement that the system of equations admits a space of operators with the basis leads to certain restrictions on the equivalent equation:

$$\begin{aligned}&\Delta_\nu=0,\\ &pr^{(2)}V_j\left[\Delta_\nu\right]=0,\end{aligned} \tag{18}$$

where $\nu=1,2$, $j=1,\ 2,\ 3,\ 4$, Δ_ν represents the different Navier–Stokes–like equation derived from different LBMs. For the Galilean transformation, we have its first-order prolongation as follows:

$$pr^{(1)}V=t\frac{\partial}{\partial x}+\frac{\partial}{\partial u}-\rho_x\frac{\partial}{\partial \rho_t}-u_x\frac{\partial}{\partial u_t}-p_x\frac{\partial}{\partial p_t}. \tag{19}$$

In this paper, the isothermal gas is considered. For this case, the equation of state reads

$$p=c_s^2\rho, \tag{20}$$

where the speed of sound, c_s, is constant. Under this consideration, we have the reduced form

$$pr^{(1)}V=t\frac{\partial}{\partial x}+\frac{\partial}{\partial u}-2\rho_x\frac{\partial}{\partial \rho_t}-u_x\frac{\partial}{\partial u_t}. \tag{21}$$

In this paper, we only present the details of the Galilean group analysis, for the others, one can derive the corresponding results in the same way. Here, the details of the analysis on the invariance of three different LBM models are presented below.

(i) One-dimensional LBE_ the 1D3Px model:[3]

$$\Delta_1\equiv\rho_t+u\rho_x+\rho u_x, \tag{22}$$

and

$$\begin{aligned}\Delta_2\equiv\ &\rho u_t+u\rho_t+\left(\frac{1}{3}+u^2\right)\rho_x+2\rho u u_x\\ &-\nu_\rho\rho_x\left(\rho u_x+u\rho_x\right)\\ &-\nu\left(\rho u_{xx}+2\rho_x u_x+u\rho_{xx}\right).\end{aligned} \tag{23}$$

The corresponding invariance equation reads:

$$\nu\rho_{xx}=-\nu_\rho\rho_x\rho_x-u\rho_x. \tag{24}$$

(ii) LBGK model:

$$\Delta_1\equiv\rho_t+u\rho_x+\rho u_x, \tag{25}$$

and

$$\Delta_2 \equiv \rho u_t + u\rho_t + u^2\rho_x + 2\rho u u_x + c_s^2\rho_x - 2\nu\left[\rho u_{xx} + 2\rho_x u_x + u\rho_{xx}\right]. \quad (26)$$

The corresponding invariance equation reads:

$$2\nu\rho_{xx} + u\rho_x = 0. \quad (27)$$

2.4. Why no invariance of Galilean transformation in one-dimensional LBM

From the theory of gas dynamics, we known that for the Navier–Stokes shock there are some inheriting constraints among the spatial derivatives, such as ρ_x, ρ_{xx}, ρ_{xxx} and so on. Table 1 shows a comparison between the group-invariant conditions for the first case, obtained from the group theoretical solution and from LBE, and we find some results in conflict with each other.

Table 1. Analysis of group-invariant conditions for the first case at shock upstream.

	ρ	ρ_x	ρ_{xx}
theoretical solution	>0	<0	<0
LBE	>0	<0	>0

The signature of the second spatial derivative of the group theory is not consistent with that obtained from LBE. So, we could see that this is the result lacking in the invariance of the Galilean transformation at the upstream of shock.

Obviously, there is no conflict in the group-invariant condition at the downstream of the shock, the sign of the second spatial derivative obtained from the group theory is the same as that obtained from the LBE. So, we can see that this is the case where the invariance of the Galilean transformation is preserved at the downstream of shock (Table 2). These group analysis results are consistent with the previous numerical results from the LBE scheme:[3] LBE scheme exhibits some momentum spikes and post-shock oscillations, meanwhile, the group-invariant condition is broken in this zone.

Table 2. Analysis of group-invariant conditions for the first case at shock downstream.

	ρ	ρ_x	ρ_{xx}
theoretical solution	>0	<0	>0
LBE	>0	<0	>0

For the second case (LBGK model), one can derive the corresponding results in the same way and obtain the same results as those obtained from one-dimensional BLE. These group analysis results are in agreement with the previous numerical results obtained from the LBGKE scheme:[5] LBGKE scheme exhibits some momentum spikes and post-shock oscillations, meanwhile, the group-invariant condition is broken in this zone. Numerical experiment shows that among the three different methods: labeled LBE, LBGK, and ELBM, only the ELBM is free from nonphysical oscillation (known as the Gibbs phenomenon in numerical analysis), which is typical of a nonentropic numerical scheme and often a portent of numerical instability.

3. Lattice Boltzmann thermohydrodynamics

3.1. Manifest Galilean covariance of LBGK model

It will appear to be a logical step to develop a microscopic approach to macroscopic phenomena by modeling the microscopic dynamics by means of a simplified description provided that the basic requirements of fundamental physics, i.e. the conservation laws and the symmetry properties, are correctly incorporated. The Galilean invariance is the basic law of classic dynamics. It should be noted that a physical LBM must inherit this symmetry. From the above analysis, we have known that in order to recover the Galilean invariance, which is not fully ensured in LBGK-gas, one may change the definition of the equation of state of the LBGK-gas. At this stage, we can set

$$\bar{c}_s = \bar{c}_s(\rho, u). \quad (28)$$

Then, the momentum equation can be rewritten as

$$\rho u_t + u\rho_t + u^2\rho_x + 2\rho u u_x = -\bar{c}_s^2\rho_x + 2\nu\left[\rho u_{xx} + 2\rho_x u_x + u\rho_{xx}\right]. \quad (29)$$

The Galilean invariance condition becomes

$$2\nu\rho_{xx} + u\rho_x - 2\bar{c}_s\frac{\partial\bar{c}_s}{\partial u}\rho_x = 0. \quad (30)$$

In order to obtain the non-oscillation solution of shock, after some algebra, one finally obtains (The details could be seen in the Appendix.)

$$\bar{c}_s^2 = RT_0 - \bar{u}u + \lambda\rho u + \frac{1}{2}u^2, \quad (31)$$

where

$$\rho(-\infty,t)=\rho_1, \tag{32}$$

$$\rho(+\infty,t)=\rho_2, \tag{33}$$

$$\lambda=\frac{8\nu}{l}\cdot\frac{1}{\rho_1-\rho_2}, \tag{34}$$

R is the constant of gas, T_0 is the reference temperature, and

$$\bar{u}=\frac{\lambda}{2}(\rho_1+\rho_2). \tag{35}$$

The equation of state reads

$$p=\rho\cdot\left(RT_0-\bar{u}u+\frac{1}{2}u^2\right)+\rho^2\cdot(\lambda u). \tag{36}$$

It should be pointed out that: according to the analysis presented in the Appendix, one can choose

$$l=\frac{4\nu}{\rho_1-\rho_2}. \tag{37}$$

Thus

$$\lambda=2. \tag{38}$$

3.2. Equation of state of LBGK-gas

The experimental pv-isotherms may be fitted over very large ranges of temperature and pressure, with a power series relation

$$pv=RT+\sum_{l=2}^{\infty}\frac{B_l(T)}{v^{l-1}}, \tag{39}$$

which is called the Virial equation of state, where T is the temperature and v is the volume. The temperature-dependent functions $B_l(T)$, $l=2,3,\ldots$, are referred to as the second, third, ... Virial coefficients. The equation of state of the LBGK-gas can be rewritten in terms of (p,v,T) as follows:

$$pv=RT+\frac{\lambda u}{v}, \tag{40}$$

where R is the gas constant and

$$RT=RT_0-\bar{u}u+\frac{1}{2}u^2. \tag{41}$$

We now use the above expression to evaluate the equation of speed. The result then can be written in the suggestive form as follows:

$$u^2-2\bar{u}u+2R(T_0-T)=0. \tag{42}$$

Hence, we have

$$u=\bar{u}\pm\sqrt{\bar{u}^2-2RT_0+2RT}. \tag{43}$$

The equation of state can be written as

$$pv=RT+\frac{\lambda}{v}\left(\bar{u}\pm\sqrt{2RT+\bar{u}^2-2RT_0}\right), \tag{44}$$

where $v=1/\rho$. In order to ensure obtaining the positive pressure, we set

$$\bar{u}^2-2RT_0=0, \tag{45}$$

and

$$u=\bar{u}+\sqrt{2RT}. \tag{46}$$

For the LBGK-gas, we have

$$B_2(T)=\lambda\cdot\sqrt{\frac{2}{RT_0}}\cdot\frac{T_0}{T}\cdot\left(1+\sqrt{\frac{T}{T_0}}\right), \tag{47}$$

and

$$B_l(T)=0,\quad l>2. \tag{48}$$

In the following thermodynamic calculation, we use

$$\begin{aligned}B(T)&\equiv\frac{B_2(T)}{RT}\\&=\left(\frac{2}{RT_0}\right)^{3/2}\cdot\left(\frac{T_0}{T}\right)^2\cdot\left(1+\sqrt{\frac{T}{T_0}}\right).\end{aligned} \tag{49}$$

At this stage, the equation of state can be rewritten as

$$p=\rho RT+2\rho^2\cdot\sqrt{\frac{2}{RT_0}}\cdot\frac{T_0}{T}\cdot\left(1+\sqrt{\frac{T}{T_0}}\right), \tag{50}$$

which is the basis of our further research of the thermodynamics of LBGK gas. We also note that the basic relation in classical thermodynamics is the equation of state, where the temperature can be well defined. However, it is not obvious how an explicit relation can be obtained in the lattice gas. This is the main trouble we faced in the previous development. We can now appreciate why the definition of a thermodynamic temperature in lattice gases (and more generally in discrete systems) in accordance with classical statistical thermodynamics is a delicate matter.

In this section, we present the closed condition in the form of equation of state from the viewpoint of Lie symmetry. Equation of state is the statement about the nature of the material in question and requires some notations from thermodynamics. Here there is no attempt to provide a rigorous derivation of the equation of state for lattice gases, such a task is beyond the scope of the traditional LBM theory. The thermal and the caloric equations of the thermodynamics are related to each other. Both are necessary for a complete thermodynamic description of a

system. The choosing of a thermal equation of state restricts the choice of a caloric equation of state but does not determine it. Note that for the Euler equations, one only requires a caloric equation of state, unless temperature is needed for some other purposes, in which case a thermal equation of state is to be given explicitly. Thermodynamic consistency requires that temperature, pressure and density changes be related through the above equation in the entire evolution of the flow.

3.3. Thermodynamic properties of LBGK-gas

During the development of LBM, the definition of a temperature in the LBM does not follow straightforwardly, and in fact it is a rather subtle matter to establish the lattice gas thermodynamics. In classical statistical thermodynamics, temperature is introduced via the canonical distribution function and the state of equation as well. The basic relation in classical thermodynamics is the equation of state, where the temperature could be well defined. However, it is not obvious how an explicit relation can be obtained in the LBGK model. In this paper, by using the invariance condition, a new equation of state is obtained, which might be analogous to the Virial expansion of the classical statistical mechanics. The deviation of the thermodynamic functions from the ideal values may be written in terms of the equation of state or the Virial coefficients. Here, we present expressions for the various functions directly in terms of the equation of state and the Virial coefficients as follows:[20]

internal energy

$$\tilde{U}-\tilde{U}^0=-\int_{\tilde{v}}^{\infty}\left\{T\left(\frac{\partial p}{\partial T}\right)_{\tilde{v}}-p\right\}\mathrm{d}\tilde{v}, \tag{51}$$

$$\tilde{U}-\tilde{U}^0=-RT\left\{\frac{T}{\tilde{v}}\frac{\mathrm{d}B}{\mathrm{d}T}\right\}; \tag{52}$$

where $\tilde{U}$ denotes internal energy per mole, $\tilde{U}^0$ represents the correction quantity compared with isothermal LBGKE. These definitions are applicable for the other thermodynamic functions presented in this section.

enthalpy

$$\begin{aligned}&\tilde{H}-\tilde{H}^0\\&=p\tilde{v}-RT-\int_{\tilde{v}}^{\infty}\left\{T\left(\frac{\partial p}{\partial T}\right)_{\tilde{v}}-p\right\}\mathrm{d}\tilde{v},\end{aligned} \tag{53}$$

$$\begin{aligned}&\tilde{H}-\tilde{H}^0\\&=RT\left\{\frac{1}{\tilde{v}}\left[B-T\frac{\mathrm{d}B}{\mathrm{d}T}\right]\right\};\end{aligned} \tag{54}$$

entropy

$$\begin{aligned}&\tilde{S}-\tilde{S}^0\\&=-R\ln p+R\ln\frac{p\tilde{v}}{RT}-\int_{\tilde{v}}^{\infty}\left[\left(\frac{\partial p}{\partial T}\right)_{\tilde{v}}-\frac{R}{\tilde{v}}\right]\mathrm{d}\tilde{v},\end{aligned} \tag{55}$$

$$\begin{aligned}&\tilde{S}-\tilde{S}^0\\&=-R\left\{\ln p+\frac{T}{\tilde{v}}\frac{\mathrm{d}B}{\mathrm{d}T}+\frac{B^2}{2\tilde{v}^2}\right\};\end{aligned} \tag{56}$$

heat capacity at constant volume

$$\tilde{C}_v-\tilde{C}_v^0=-T\int_{\tilde{v}}^{\infty}\left(\frac{\partial^2 p}{\partial T^2}\right)_{\tilde{v}}\mathrm{d}\tilde{v}, \tag{57}$$

$$\tilde{C}_v-\tilde{C}_v^0=-R\left\{\frac{2T}{\tilde{v}}\frac{\mathrm{d}B}{\mathrm{d}T}+\frac{T^2}{\tilde{v}}\frac{\mathrm{d}^2B}{\mathrm{d}T^2}\right\}; \tag{58}$$

heat capacity at constant pressure

$$\begin{aligned}&\tilde{C}_p-\tilde{C}_p^0\\&=-R-\frac{T\left(\frac{\partial p}{\partial T}\right)_{\tilde{v}}^2}{\left(\frac{\partial p}{\partial\tilde{v}}\right)_T}-T\int_{\tilde{v}}^{\infty}\left(\frac{\partial^2 p}{\partial T^2}\right)_{\tilde{v}}\mathrm{d}\tilde{v},\end{aligned} \tag{59}$$

$$\begin{aligned}&\tilde{C}_p-\tilde{C}_p^0\\&=-R\left\{\frac{T^2}{\tilde{v}}\frac{\mathrm{d}^2B}{\mathrm{d}T^2}-\frac{1}{\tilde{v}^2}\left[\left(B-T\frac{\mathrm{d}B}{\mathrm{d}T}\right)^2\right]\right\};\end{aligned} \tag{60}$$

Joule–Thomson coefficient

$$\begin{aligned}&\mu\\&=\frac{1}{\tilde{C}_p}\left[T\left(\frac{\partial\tilde{v}}{\partial T}\right)_P-\tilde{v}\right],\end{aligned} \tag{61}$$

$$\begin{aligned}&\mu\\&=-\frac{1}{\tilde{C}_p^0}\left\{T\frac{\mathrm{d}B}{\mathrm{d}T}-B+\frac{1}{\tilde{v}}\left[\left(2B^2-T\frac{\mathrm{d}B}{\mathrm{d}T}\right)^2\right]\right\};\end{aligned} \tag{62}$$

speed of sound

$$c_0^2=-\frac{\gamma v^2}{M}\left(\frac{\partial p}{\partial\tilde{v}}\right)_T, \tag{63}$$

$$\begin{aligned}c_0^2=&\frac{\gamma^0RT}{M}\left\{1+\frac{1}{\tilde{v}}\left[2B+2\left(\gamma^0-1\right)T\frac{\mathrm{d}B}{\mathrm{d}T}\right.\right.\\&\left.\left.+\frac{\left(\gamma^0-1\right)^2}{\gamma^0}T^2\frac{\mathrm{d}^2B}{\mathrm{d}T^2}\right]\right\},\end{aligned} \tag{64}$$

in which $\gamma=\tilde{C}_p/\tilde{C}_v$.

From the above expressions, we can see that the theoretical expressions for the various functions are directly described in terms of the equation of state and the Virial coefficients. However, it is a very difficult task in the former theoretical development.

4. Conclusions

In the present paper, a rigorous systematic method is established for the invariance analysis of the typical LBGK model. The invariance, especially Galilean invariance, has been an important issue in lattice-based hydrodynamics models. The previous models concentrated on the nonlinear advection term and stressed that Galilean invariance was a basic requirement for any physical model. In the present paper, we consider this fundamental problem about LBGK to study the high speed flows, from the viewpoint of group invariance. The main results obtained in this paper reveal that there seems to be some inherent connection between the Galilean invariance and the natural thermal hydrodynamics. The equation of state can be deduced from this symmetry analysis. Lie symmetry consideration completes the description of the LBGK model for isothermal Navier–Stokes equation as a self–contained kinetic theory admitting a proper equation of state. The corresponding theory for its thermo-hydrodynamics is naturally deduced, which is compatible with the elementary statistical thermodynamics. How to use these new findings to improve the LBM for high speed flows will be seen in our further publications.[21]

Appendix: Travelling wave solution of Burgers equation

In general, traveling wave solutions to a partial differential equation arise as special group-invariant solutions in which the group under consideration is a translation group in the space of independent variables. Here we consider Burgers equation

$$\bar{W}_t + \bar{W}\bar{W}_x = \nu \bar{W}_{xx}. \tag{A1}$$

In terms of the invariant

$$y = x - ct, \tag{A2}$$

the reduced equation is

$$-c\bar{W}_y + \bar{W}\bar{W}_y - \nu \bar{W}_{yy} = 0. \tag{A3}$$

The general solution can be written in terms of hyperbolic function as

$$\bar{W}(x,t) = \frac{\bar{W}_1 + \bar{W}_2}{2} - \frac{\bar{W}_1 - \bar{W}_2}{2} \tanh\left[\frac{\bar{W}_1 - \bar{W}_2}{4\nu} \cdot (x - ct)\right], \tag{A4}$$

where

$$\bar{W}(-\infty, t) = \bar{W}_1, \tag{A5}$$

$$\bar{W}(+\infty, t) = \bar{W}_2, \tag{A6}$$

and

$$c = \frac{\bar{W}_1 + \bar{W}_2}{2}. \tag{A7}$$

Acoording to the general solution of Burgers equation (A1), we set

$$\rho(x,t) = \frac{\rho_1 + \rho_2}{2} - \frac{\rho_1 - \rho_2}{2} \tanh\left[\frac{1}{l} \cdot (x - ct)\right], \tag{A8}$$

where

$$\rho(-\infty, t) = \rho_1, \tag{A9}$$

and

$$\rho(+\infty, t) = \rho_2. \tag{A10}$$

It is easy to prove that

$$\frac{\rho_{xx}}{\rho_x} = \frac{4}{l(\rho_1 - \rho_2)} \cdot \left(\rho - \frac{\rho_1 + \rho_2}{2}\right). \tag{A11}$$

The Galilean invariance condition becomes

$$\frac{\partial}{\partial u}\left[\bar{c}_s^2 - \frac{1}{2}u^2\right] = \lambda\left(\rho - \frac{\rho_1 + \rho_2}{2}\right), \tag{A12}$$

where

$$\lambda = \frac{8\nu}{l} \cdot \frac{1}{\rho_1 - \rho_2}. \tag{A13}$$

The general solution can be written as

$$\bar{c}_s^2 = RT_0 - \bar{u}u + \lambda\rho u + \frac{1}{2}u^2, \tag{A14}$$

where R is the constant of gas, T_0 is the reference temperature, and

$$\bar{u} = \frac{\lambda}{2}\left(\rho_1 + \rho_2\right). \tag{A15}$$

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