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Theory of the lattice Boltzmann method: From the Boltzmann equation to the lattice Boltzmann equation

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In this paper, the lattice Boltzmann equation is directly derived from the Boltzmann equation. It is shown that the lattice Boltzmann equation is a special discretized form of the Boltzmann equation. Various approximations for the discretization of the Boltzmann equation in both time and phase space are discussed in detail. A general procedure to derive the lattice Boltzmann model from the continuous Boltzmann equation is demonstrated explicitly. The lattice Boltzmann models derived include the two-dimensional 6-bit, 7-bit, and 9-bit, and three-dimensional 27-bit models. [S1063-651X(97)12512-0]

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I. INTRODUCTION

In the last few years, we have witnessed a rapid development of the method known as the lattice Boltzmann equation (LBE) [1–6]. Although only in its infancy, the LBE method has demonstrated its ability to simulate hydrodynamic systems [1–5], magnetohydrodynamic systems [7], multiphase and multicomponent fluids [8] including suspensions [9] and emulsions [10], chemical-reactive flows [11], and multicomponent flow through porous media [12]. Together with modern computers of massively parallel processors, the LBE method has become a powerful computational method for studying various complex systems. The obvious advantages of the LBE method are the parallelism of the method, the simplicity of the programming, and the capability of incorporating model interactions. However, a rigorous framework of the LBE method is still lacking in spite of the great interest in the method.

Historically, the models of the lattice Boltzmann equation directly evolve from the models of the lattice-gas automata (LGA) [13]. While the LGA models are Boolean ones, the LBE models are indeed the floating-number counterpart of the corresponding LGA models—a particle in the LGA model (represented by a Boolean number) is replaced by the single-particle distribution function (represented by a real number). Even though the LBE models appear to be rather different from their LGA counterparts because various approximations, such as the linearization of the collision operator [2] and the Bhatnagar-Gross-Krook (BGK) [15–17] approximation [3], have been applied, the theoretical framework of the LBE method nevertheless rests upon the Chapman-Enskog analysis of the LGA method [14]. Although the connection between the LBE models and the continuous Boltzmann equation are discussed in various places [18,19], so far there exists no rigorous result in this direction. The lack of a thorough understanding of the LBE method has some immediate implications. For instance, the LBE method has not been very successful in simulating thermohydrodynamic systems [19–22], nor has the LBE method been able to be implemented on arbitrary mesh grids [5,23], even though considerable effort has been applied in these directions. As we have shown recently [24–26], substantial progress can be made in the aforementioned areas once a better understanding of the LBE method is attained. Furthermore, through the derivation we can directly show the connection between the LBE method and other newly developed gas kinetic methods [27–33].

In this paper we will show that the lattice Boltzmann equation can be directly derived from the continuous Boltzmann equation discretized in some special manner in both time and phase space. Our analysis shows that theoretically the lattice Boltzmann equation is independent of the lattice-gas automata. The lattice Boltzmann equation is a finite-difference form of the continuous Boltzmann equation. We provide a detailed account of an *a priori* derivation of the lattice Boltzmann equation from its continuous counterpart—the continuous Boltzmann equation. A general procedure to derive lattice Boltzmann models from the continuous Boltzmann equation is established. A number of LBE models in both two- and three-dimensional (2D, 3D) space are derived to illustrate the procedure. The kinetic-model equation used in this paper is the BGK equation with a single relaxation time [15–17]. Although the BGK equation has its inherent limitations and shortcomings, such as fixed Prandtl number, the equation can be generalized to remedy the shortcomings [34]. Therefore, it is sufficient to use the BGK equation for the purpose of studying hydrodynamics of simple fluids.

This paper is organized as follows. In Sec. II we discuss the discretization of time for the Boltzmann BGK equation. In Sec. III we discuss the low Mach number (small velocity) expansion and the discretization of the phase space. In Sec. IV we derive the lattice Boltzmann 6-bit, 7-bit, and 9-bit models in two-dimensional space and the 27-bit model in three-dimensional space. Section V concludes the paper.

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II. DISCRETIZATION OF THE BOLTZMANN EQUATION

In the following analysis, we shall use the Boltzmann equation with the BGK, or single-relaxation-time, approximation [15–17]:

$$\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\nabla f=-\frac{1}{\lambda}(f-g), \tag{1}$$

where $f\equiv f(\boldsymbol{x},\boldsymbol{\xi},t)$ is the single-particle distribution function, $\boldsymbol{\xi}$ is the microscopic velocity, λ is the relaxation time due to collision, and g is the Boltzmann-Maxwellian distribution function:

$$g\equiv\frac{\rho}{(2\pi RT)^{D/2}}\exp\left(-\frac{(\boldsymbol{\xi}-\boldsymbol{u})^2}{2RT}\right), \tag{2}$$

where R is the ideal gas constant, D is the dimension of the space, and ρ, $\boldsymbol{u}$, and T are the macroscopic density of mass, velocity, and temperature, respectively. The macroscopic variables, ρ, $\boldsymbol{u}$, and T are the (microscopic velocity) moments of the distribution function, f:

$$\rho=\int f d\boldsymbol{\xi}=\int g d\boldsymbol{\xi}, \tag{3a}$$

$$\rho\boldsymbol{u}=\int \boldsymbol{\xi} f d\boldsymbol{\xi}=\int \boldsymbol{\xi} g d\boldsymbol{\xi}, \tag{3b}$$

$$\rho\varepsilon=\frac{1}{2}\int(\boldsymbol{\xi}-\boldsymbol{u})^2 f d\boldsymbol{\xi}=\frac{1}{2}\int(\boldsymbol{\xi}-\boldsymbol{u})^2 g d\boldsymbol{\xi}. \tag{3c}$$

The energy can also be written in terms of temperature T:

$$\varepsilon=\frac{D_0}{2}RT=\frac{D_0}{2}N_A k_B T, \tag{4}$$

where D_0, N_A, and k_B are the number of degrees of freedom of a particle, Avogadro's number, and the Boltzmann constant, respectively. In Eqs. (3), an assumption of Chapman-Enskog [16] has been applied:

$$\int h(\boldsymbol{\xi})f(\boldsymbol{x},\boldsymbol{\xi},t)d\boldsymbol{\xi}=\int h(\boldsymbol{\xi})g(\boldsymbol{x},\boldsymbol{\xi},t)d\boldsymbol{\xi}, \tag{5}$$

where $h(\xi)$ is a linear combination of collisional invariants (conserved quantities)

$$h(\boldsymbol{\xi})=A+\boldsymbol{B}\cdot\boldsymbol{\xi}+C\boldsymbol{\xi}\cdot\boldsymbol{\xi}. \tag{6}$$

In the above equation, A and C are arbitrary constants, and $\boldsymbol{B}$ is an arbitrary constant vector.

A. Discretization of time

Equation (1) can be formally rewritten in the form of an ordinary differential equation:

$$\frac{df}{dt}+\frac{1}{\lambda}f=\frac{1}{\lambda}g, \tag{7}$$

where

$$\frac{d}{dt}\equiv\frac{\partial}{\partial t}+\boldsymbol{\xi}\cdot\boldsymbol{\nabla}$$

is the time derivative along the characteristic line $\boldsymbol{\xi}$. The above equation can be formally integrated over a time step of δ_t:

$$f(\boldsymbol{x}+\boldsymbol{\xi}\delta_t,\boldsymbol{\xi},t+\delta_t)=\frac{1}{\lambda}e^{-\delta_t/\lambda}\int_0^{\delta_t}e^{t'/\lambda}g(\boldsymbol{x}+\boldsymbol{\xi}t',\boldsymbol{\xi},t+t')dt' + e^{-\delta_t/\lambda}f(\boldsymbol{x},\boldsymbol{\xi},t). \tag{8}$$

Assuming that δ_t is small enough and g is smooth enough locally, the following approximation can be made:

$$g(\boldsymbol{x}+\boldsymbol{\xi}t',\boldsymbol{\xi},t+t')=\left(1-\frac{t'}{\delta_t}\right)g(\boldsymbol{x},\boldsymbol{\xi},t) + \frac{t'}{\delta_t}g(\boldsymbol{x}+\boldsymbol{\xi}\delta_t,\boldsymbol{\xi},t+\delta_t) + O(\delta_t^2), \quad 0\leqslant t'\leqslant\delta_t. \tag{9}$$

The leading terms neglected in the above approximation are of the order of $O(\delta_t^2)$. With this approximation, Eq. (8) becomes

$$\begin{aligned} f(\boldsymbol{x}+\boldsymbol{\xi}\delta_t,\boldsymbol{\xi},t+\delta_t)-f(\boldsymbol{x},\boldsymbol{\xi},t) &=(e^{-\delta_t/\lambda}-1)[f(\boldsymbol{x},\boldsymbol{\xi},t)-g(\boldsymbol{x},\boldsymbol{\xi},t)] \\ &+\left(1+\frac{\lambda}{\delta_t}(e^{-\delta_t/\lambda}-1)\right) \\ &\times[g(\boldsymbol{x}+\boldsymbol{\xi}\delta_t,\boldsymbol{\xi},t+\delta_t)-g(\boldsymbol{x},\boldsymbol{\xi},t)]. \end{aligned} \tag{10}$$

If we expand $e^{-\delta_t/\lambda}$ in its Taylor expansion and, further, neglect the terms of order $O(\delta_t^2)$ or smaller on the right-hand side of Eq. (10), then Eq. (10) becomes

$$f(\boldsymbol{x}+\boldsymbol{\xi}\delta_t,\boldsymbol{\xi},t+\delta_t)-f(\boldsymbol{x},\boldsymbol{\xi},t)=-\frac{1}{\tau}[f(\boldsymbol{x},\boldsymbol{\xi},t)-g(\boldsymbol{x},\boldsymbol{\xi},t)], \tag{11}$$

where $\tau\equiv\lambda/\delta_t$ is the dimensionless relaxation time (in the unit of δ_t). Therefore, Eq. (11) is accurate to the first order in δ_t. Equation (11) is the evolution equation of the distribution function f with discrete time.

Although g is written as an explicit function of t, the time dependence of g lies solely in the hydrodynamic variables ρ, $\boldsymbol{u}$, and T (the Chapman-Enskog ansatz [16]), that is, $g(\boldsymbol{x},\boldsymbol{\xi},t)=g(\boldsymbol{x},\boldsymbol{\xi};\rho,\boldsymbol{u},T)$. Therefore, one must first compute ρ, $\boldsymbol{u}$, and T before constructing the equilibrium distribution function, g. Thus, the calculation of ρ, $\boldsymbol{u}$, and T becomes one of the most crucial steps in discretizing the Boltzmann equation.

B. Calculation of the hydrodynamic moments

In order to numerically evaluate the hydrodynamic moments of Eq. (3), appropriate discretization in momentum space $\boldsymbol{\xi}$ must be accomplished. With appropriate discretization, integration in momentum space (with weight function g) can be approximated by quadrature up to a certain degree of accuracy, that is,

$$\int \psi(\boldsymbol{\xi}) g(\boldsymbol{x},\xi,t) d\boldsymbol{\xi} = \sum_\alpha W_\alpha \psi(\boldsymbol{\xi}_\alpha) g(\boldsymbol{x},\boldsymbol{\xi}_\alpha,t), \quad (12)$$

where $\psi(\boldsymbol{\xi})$ is a polynomial of $\boldsymbol{\xi}$, W_α is the weight coefficient of the quadrature, and $\boldsymbol{\xi}_\alpha$ is the discrete velocity set or the abscissas of the quadrature. Accordingly, the hydrodynamic moments of Eqs. (3) can be computed by

$$\rho = \sum_\alpha f_\alpha = \sum_\alpha g_\alpha, \quad (13a)$$

$$\rho \boldsymbol{u} = \sum_\alpha \boldsymbol{\xi}_\alpha f_\alpha = \sum_\alpha \boldsymbol{\xi}_\alpha g_\alpha, \quad (13b)$$

$$\rho\varepsilon = \frac{1}{2}\sum_\alpha (\boldsymbol{\xi}_\alpha - \boldsymbol{u})^2 f_\alpha = \frac{1}{2}\sum_\alpha (\boldsymbol{\xi}_\alpha - \boldsymbol{u})^2 g_\alpha, \quad (13c)$$

where

$$f_\alpha \equiv f_\alpha(\boldsymbol{x},t) \equiv W_\alpha f(\boldsymbol{x},\boldsymbol{\xi}_\alpha,t), \quad (14a)$$

$$g_\alpha \equiv g_\alpha(\boldsymbol{x},t) \equiv W_\alpha g(\boldsymbol{x},\boldsymbol{\xi}_\alpha,t). \quad (14b)$$

It should also be noted that f_α (or g_α) has the unit of $f d\boldsymbol{\xi}$ (or $g d\boldsymbol{\xi}$).

III. DERIVATION OF THE LATTICE BOLTZMANN EQUATION AND ITS EQUILIBRIUM DISTRIBUTION FUNCTION

The lattice Boltzmann equation has the following ingredients: (1) an evolution equation, in the form of Eq. (11) with discretized time and phase space of which configuration space is of a lattice structure and momentum space is reduced to a small set of discrete momenta; (2) conservation constraints in the form of Eq. (13); (3) a proper equilibrium distribution function which leads to the Navier-Stokes equations. In what follows, the low Mach number expansion is first applied to the Boltzmann-Maxwellian distribution function. Then quadrature to approximate the integration in the momentum space $\boldsymbol{\xi}$ is discussed in detail for a variety of LBE models in both 2D and 3D space. Through the quadrature, the lattice structure, and the equilibrium distribution function of the LBE are constructed.

A. Low-Mach-number approximation

In the lattice Boltzmann equation, the equilibrium distribution function is obtained by a truncated small velocity expansion (or low-Mach-number approximation) [14]. The same can be done here:

$$g = \frac{\rho}{(2\pi RT)^{D/2}} \exp(-\boldsymbol{\xi}^2/2RT) \exp\{(\boldsymbol{\xi}\cdot\boldsymbol{u})/RT - \boldsymbol{u}^2/2RT\}$$
$$= \frac{\rho}{(2\pi RT)^{D/2}} \exp(-\boldsymbol{\xi}^2/2RT) \times\left\{1 + \frac{(\boldsymbol{\xi}\cdot\boldsymbol{u})}{RT} + \frac{(\boldsymbol{\xi}\cdot\boldsymbol{u})^2}{2(RT)^2} - \frac{\boldsymbol{u}^2}{2RT}\right\} + O(\boldsymbol{u}^3). \quad (15)$$

With the equilibrium distribution function g of the above form, Eq. (11) bears a strong resemblance to the lattice Boltzmann equation, and what remains to be accomplished is the discretization of phase space. For convenience, the following notation for the equilibrium distribution function with truncated small velocity expansion shall be used in what follows:

$$f^{(\mathrm{eq})} = \frac{\rho}{(2\pi RT)^{D/2}} \exp(-\boldsymbol{\xi}^2/2RT) \times\left\{1 + \frac{(\boldsymbol{\xi}\cdot\boldsymbol{u})}{RT} + \frac{(\boldsymbol{\xi}\cdot\boldsymbol{u})^2}{2(RT)^2} - \frac{\boldsymbol{u}^2}{2RT}\right\}. \quad (16)$$

Although $f^{(\mathrm{eq})}$ only retains the terms up to $O(\boldsymbol{u}^2)$, it is trivial to maintain high-order terms of $\boldsymbol{u}$ in the above expansion if necessary.

B. Discretization of phase space

There are two considerations in the discretization of phase space. First of all, the discretization of momentum space is coupled to that of configuration space such that a lattice structure is obtained. This is a special characteristic of the lattice Boltzmann equation. Second, the quadrature must be accurate enough so that not only the conservation constraints of Eq. (13) are preserved exactly, but also the necessary symmetries required by the Navier-Stokes equations are retained.

In deriving the Navier-Stokes equations from the Boltzmann equation via the Chapman-Enskog analysis [16,17], the first two order approximations of the distribution function (i.e., $f^{(\mathrm{eq})}$ and $f^{(1)}$) must be considered. Therefore, given the equilibrium distribution function, $f^{(\mathrm{eq})}$ of Eq. (16), the quadrature used to evaluate the hydrodynamic moments must be able to compute the following moments with respect to $f^{(\mathrm{eq})}$ exactly:

$$\rho: \quad 1, \xi_i, \ \xi_i\xi_j, \quad (17a)$$

$$\boldsymbol{u}: \quad \xi_i, \ \xi_i\xi_j, \ \xi_i\xi_j\xi_k, \quad (17b)$$

$$T: \quad \xi_i\xi_j, \ \xi_i\xi_j\xi_k, \ \xi_i\xi_j\xi_k\xi_l, \quad (17c)$$

where ξ_i is the component of $\boldsymbol{\xi}$ in Cartesian coordinates. (We have assumed that the particle only has the linear degree of freedom, i.e., $D_0 = D$.) Thus, to obtain the Navier-Stokes equations, one must be able to evaluate the moments of 1, $\boldsymbol{\xi},\ldots,\boldsymbol{\xi}^6$ with respect to weight function $\exp(-\boldsymbol{\xi}^2/2RT)$ exactly, owing to the small $\boldsymbol{u}$ expansion of g. For isothermal models, which are discussed in what follows, the moments that are to be evaluated are 1, $\boldsymbol{\xi},\ldots,\boldsymbol{\xi}^5$.

Calculating the hydrodynamic moments of $f^{(\mathrm{eq})}$ is equivalent to evaluating the following integral in general:

$$I = \int \psi(\boldsymbol{\xi}) f^{(\mathrm{eq})} d\boldsymbol{\xi} = \frac{\rho}{(2\pi RT)^{D/2}} \int \psi(\boldsymbol{\xi}) \exp(-\boldsymbol{\xi}^2/2RT) \times\left\{1 + \frac{(\boldsymbol{\xi}\cdot\boldsymbol{u})}{RT} + \frac{(\boldsymbol{\xi}\cdot\boldsymbol{u})^2}{2(RT)^2} - \frac{\boldsymbol{u}^2}{2RT}\right\} d\boldsymbol{\xi}, \quad (18)$$

where $\psi(\boldsymbol{\xi})$ is a polynomial of $\boldsymbol{\xi}$. The above integral has the following structure:

$$\int e^{-x^2}\psi(x)dx,$$

which can be calculated numerically with Gaussian-type quadrature [35]. Our objective is to use quadrature to evaluate the hydrodynamic moments [ρ, $\boldsymbol{u}$, and T, given by Eq. (3)]. Given proper discretization of phase space, we can evaluate the above integral with desirable accuracy. In the meantime, the lattice Boltzmann equation with appropriate equilibrium distribution function can also be derived.

IV. LATTICE BOLTZMANN MODELS IN TWO- AND THREE-DIMENSIONAL SPACE

A. Two-dimensional 6-bit and 7-bit triangular lattice model

The 7-bit model is constructed on a two-dimensional ($D=2$) triangular lattice space. The triangular lattice has the necessary rotational symmetry required by the hydrodynamics [14]. The polar coordinates of $\boldsymbol{\xi}$ space, (ξ, θ), are used here. For the sake of simplicity but without losing generality, assuming

$$\psi_{m,n}(\boldsymbol{\xi})=(\sqrt{2RT})^{m+n}\zeta^{m+n}\cos^m\theta\,\sin^n\theta, \tag{19}$$

where $\zeta=\xi/\sqrt{2RT}$, the integral in Eq. (18) becomes

$$I=\int\psi_{m,n}(\boldsymbol{\xi})f^{(\mathrm{eq})}d\boldsymbol{\xi}$$
$$=\frac{\rho}{\pi}(\sqrt{2RT})^{m+n}\int_0^{2\pi}\int_0^{\infty}e^{-\zeta^2}\zeta^{m+n}\cos^m\theta\,\sin^n\theta$$
$$\times\left\{1+\frac{2\zeta(\hat{\boldsymbol{e}}\cdot\boldsymbol{u})}{\sqrt{2RT}}+\frac{\zeta^2(\hat{\boldsymbol{e}}\cdot\boldsymbol{u})^2}{RT}-\frac{\boldsymbol{u}^2}{2RT}\right\}d\theta\zeta d\zeta, \tag{20}$$

where $\hat{e}=(\cos\theta, \sin\theta)$. To obtain the 7-bit lattice Boltzmann equation on the triangular lattice space, the angular variable θ must be discretized evenly into six sections in the interval $[0, 2\pi)$, that is, $\theta_\alpha=(\alpha-1)\pi/3$, for $\alpha=\{1,2,...,6\}$. With the discretization of θ, we have

$$\int_0^{2\pi}\cos^m\theta\,\sin^n\theta d\theta$$
$$=\begin{cases}\dfrac{\pi}{3}\displaystyle\sum_{\alpha=1}^{6}\cos^m\theta_\alpha\,\sin^n\theta_\alpha, & (m+n)\ \text{even}\\ 0, & (m+n)\ \text{odd}\end{cases} \tag{21}$$

for $(m+n)\leqslant 5$. Using the above result, we obtain

$$I=\begin{cases}\dfrac{\rho}{3}(\sqrt{2RT})^{m+n}\displaystyle\sum_{\alpha=1}^{6}\cos^m\theta_\alpha\,\sin^n\theta_\alpha\left\{\left(1-\frac{\boldsymbol{u}^2}{2RT}\right)I_{m+n}+\frac{(\hat{\boldsymbol{e}}_\alpha\cdot\boldsymbol{u})^2}{RT}I_{m+n+2}\right\}, & (m+n)\ \text{even}\\ \dfrac{\rho}{3}(\sqrt{2RT})^{m+n}\displaystyle\sum_{\alpha=1}^{6}\cos^m\theta_\alpha\,\sin^n\theta_\alpha\frac{2(\hat{\boldsymbol{e}}_\alpha\cdot\boldsymbol{u})}{\sqrt{2RT}}I_{m+n+1}, & (m+n)\ \text{odd,}\end{cases} \tag{22}$$

where $\hat{e}_\alpha=(\cos\theta_\alpha, \sin\theta_\alpha)$, and

$$I_m=\int_0^{+\infty}(\zeta e^{-\zeta^2})\zeta^m d\zeta \tag{23}$$

is the mth moment with respect to the weight function $\zeta e^{-\zeta^2}$.

Since the 7-bit model only has two speeds (i.e., $n=2$) and one of them is fixed at 0, it is clear that the abscissas of the quadrature to evaluate I_m should be $\zeta_0=0$ and $\zeta_1=\gamma^{-1}$, where γ is a positive parameter to be adjusted later. The Radau-Gauss formula [35] is a natural choice to evaluate the integral I_m:

$$I_m=\omega_0\zeta_0^m+\sum_{j=1}^{n}\omega_j\zeta_j^m.$$

For the 7-bit model, $n=1$, and the integrals needed to be evaluated are I_0, I_2, and I_4. [I_1 and I_3 do not play any role because of the symmetry of the integral I, as shown in Eq. (22).] Then, we have the following three equations:

$$I_0=\omega_0+\omega_1=1/2, \tag{24a}$$

$$I_2=\omega_1\gamma^{-2}=1/2, \tag{24b}$$

$$I_4=\omega_1\gamma^{-4}=1, \tag{24c}$$

of which, the solutions are

$$\omega_0=1/4, \tag{25a}$$

$$\omega_1=1/4, \tag{25b}$$

$$\gamma=1/\sqrt{2}. \tag{25c}$$

Therefore, we have

$$I_m=\tfrac{1}{4}(\zeta_0^m+\zeta_1^m),\quad m=0,2,4. \tag{26}$$

Note that the above quadrature for I_m is *exact* for $m=0$, 2, and 4. Consequently, the following equality is expected to be exact for $(m+n)\leqslant 5$:

$$I=\frac{\rho}{12}(\sqrt{2RT})^{m+n}\sum_{\alpha=1}^{6}\cos^m\theta_\alpha\sin^n\theta_\alpha\left\{\left(1-\frac{\boldsymbol{u}^2}{2RT}\right)\right.$$
$$\times(\zeta_0^{m+n}+\zeta_1^{m+n})+\frac{2(\hat{\boldsymbol{e}}_\alpha\cdot\boldsymbol{u})}{\sqrt{2RT}}(\zeta_0^{m+n+1}+\zeta_1^{m+n+1})$$
$$\left.+\frac{(\hat{\boldsymbol{e}}_\alpha\cdot\boldsymbol{u})^2}{RT}(\zeta_0^{m+n+2}+\zeta_1^{m+n+2})\right\}$$
$$=\frac{\rho}{2}\psi_{m,n}(\boldsymbol{\xi}_0)\left\{1-\frac{\boldsymbol{u}^2}{2RT}\right\}+\frac{\rho}{12}\sum_{\alpha=1}^{6}\psi_{m,n}(\boldsymbol{\xi}_\alpha)$$
$$\times\left\{1+\frac{(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})}{RT}+\frac{(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})^2}{2(RT)^2}-\frac{\boldsymbol{u}^2}{2RT}\right\},$$

where $\|\boldsymbol{\xi}_0\|=\sqrt{2RT}\zeta_0=0$ and $\boldsymbol{\xi}_\alpha=\sqrt{2RT}\zeta_1\hat{\boldsymbol{e}}_\alpha=2\sqrt{RT}\hat{\boldsymbol{e}}_\alpha$. It becomes obvious that the equilibrium distribution function for the 7-bit model is

$$f_\alpha^{(\mathrm{eq})}=w_\alpha\rho\left\{1+\frac{4(\boldsymbol{e}_\alpha\cdot\boldsymbol{u})}{c^2}+\frac{8(\boldsymbol{e}_\alpha\cdot\boldsymbol{u})^2}{c^4}-\frac{2\boldsymbol{u}^2}{c^2}\right\}, \tag{27}$$

where $\alpha\in\{0,1,2,...,6\}$,

$$c=\frac{\delta_x}{\delta_t} \tag{28}$$

is "the speed of light" in the system (which is usually set to be unity in the literature),

$$\boldsymbol{e}_\alpha=\begin{cases}(0,0), & \alpha=0\\ (\cos\theta_\alpha,\sin\theta_\alpha)c,\quad \theta_\alpha=(\alpha-1)\pi/3, & \alpha=1,2,...,6\end{cases} \tag{29}$$

and

$$w_\alpha=\begin{cases}1/2, & \alpha=0\\ 1/12, & \alpha=1,2,...,6.\end{cases} \tag{30}$$

Note that the substitution of $RT=c_s^2=c^2/4$, where c_s is the sound speed of the system, has been made in Eq. (27), and $RT=c_s^2=c^2/4$ is equivalent to $\|\boldsymbol{\xi}_\alpha\|=c$ for $\alpha\neq0$. The coefficient W_α defined in Eq. (14) is explicitly given by

$$W_\alpha=(2\pi RT)^{D/2}e^{\xi_\alpha^2/2RT}w_\alpha. \tag{31}$$

Similarly, the equilibrium distribution function for the 6-bit LBE model, which is a degenerate case of the 7-bit model, can be obtained easily by solving two equations for one abscissa and the weight coefficient of the Hermite-Gauss formula [35] with modification for the integral on half real axis [36]. The solutions are $\omega_1=\frac{1}{2}$ and $\gamma=1$. Then, we have

$$f_\alpha^{(\mathrm{eq})}=\frac{\rho}{6}\left\{1+\frac{2(\boldsymbol{e}_\alpha\cdot\boldsymbol{u})}{c^2}+\frac{4(\boldsymbol{e}_\alpha\cdot\boldsymbol{u})^2}{c^4}-\frac{\boldsymbol{u}^2}{c^2}\right\}, \tag{32}$$

where $\alpha\in\{1,2,...,6\}$. The sound speed of the 6-bit LBE model is $c_s=c/\sqrt{2}$, and $w_\alpha=\frac{1}{6}$.

B. Two-dimensional 9-bit square lattice model

To recover the 9-bit LBE model on square lattice space, the Cartesian coordinate system is used and, accordingly, $\psi(\boldsymbol{\xi})$ can be set to

$$\psi_{m,n}(\boldsymbol{\xi})=\xi_x^m\xi_y^n,$$

where ξ_x and ξ_y are the x and y components of $\boldsymbol{\xi}$. The integral of the moments, defined by Eq. (18), becomes

$$I=\int\psi_{m,n}(\boldsymbol{\xi})f^{(\mathrm{eq})}d\boldsymbol{\xi}=\frac{\rho}{\pi}(\sqrt{2RT})^{m+n}\left\{\left(1-\frac{\boldsymbol{u}^2}{2RT}\right)I_mI_n\right.$$
$$+\frac{2(u_xI_{m+1}I_n+u_yI_mI_{n+1})}{\sqrt{2RT}}$$
$$\left.+\frac{u_x^2I_{m+2}I_n+2u_xu_yI_{m+1}I_{n+1}+u_y^2I_mI_{n+2}}{RT}\right\}, \tag{33}$$

where

$$I_m=\int_{-\infty}^{+\infty}e^{-\zeta^2}\zeta^m d\zeta,\quad \zeta=\xi/\sqrt{2RT}$$

is the mth order moment of the weight function $e^{-\zeta^2}$ on the real axis. Naturally, the third-order Hermite formula [35] is the optimal choice to evaluate I_m for the purpose of deriving the 9-bit LBE model:

$$I_m=\sum_{j=1}^{3}\omega_j\zeta_j^m.$$

The three abscissas of the quadrature are

$$\zeta_1=-\sqrt{3/2},\quad \zeta_2=0,\quad \zeta_3=\sqrt{3/2}, \tag{34}$$

and the corresponding weight coefficients are

$$\omega_1=\sqrt{\pi}/6,\quad \omega_2=2\sqrt{\pi}/3,\quad \omega_3=\sqrt{\pi}/6. \tag{35}$$

Then, the integral of the moment in Eq. (33) becomes

$$I=\frac{\rho}{\pi}\sum_{i,j=1}^{3}\omega_i\omega_j\psi(\boldsymbol{\xi}_{i,j})\left\{1+\frac{(\boldsymbol{\xi}_{i,j}\cdot\boldsymbol{u})}{RT}+\frac{(\boldsymbol{\xi}_{i,j}\cdot\boldsymbol{u})^2}{2(RT)^2}-\frac{\boldsymbol{u}^2}{2RT}\right\}, \tag{36}$$

where $\boldsymbol{\xi}_{i,j}=(\xi_i,\xi_j)=\sqrt{2RT}(\zeta_i,\zeta_j)$. Obviously, we can identify the equilibrium distribution function with

$$f_{i,j}^{(\mathrm{eq})}=\frac{\omega_i\omega_j}{\pi}\rho\left\{1+\frac{(\boldsymbol{\xi}_{i,j}\cdot\boldsymbol{u})}{RT}+\frac{(\boldsymbol{\xi}_{i,j}\cdot\boldsymbol{u})^2}{2(RT)^2}-\frac{\boldsymbol{u}^2}{2RT}\right\}. \tag{37}$$

Employing the notations of

$$e_\alpha=\begin{cases}(0,0), & & \alpha=0\\ (\cos\theta_\alpha,\ \sin\theta_\alpha)c, & \theta_\alpha=(\alpha-1)\pi/2, & \alpha=1,2,3,4\\ \sqrt{2}(\cos\theta_\alpha,\ \sin\theta_\alpha)c, & \theta_\alpha=(\alpha-5)\pi/2+\pi/4, & \alpha=5,6,7,8\end{cases}\tag{38}$$

and

$$w_\alpha=\frac{\omega_i\omega_j}{\pi}=\begin{cases}4/9, & i=j=2, & \alpha=0\\ 1/9, & i=1,\ j=2,\ \ldots, & \alpha=1,2,3,4\\ 1/36, & i=j=1,\ \ldots, & \alpha=5,6,7,8,\end{cases}\tag{39}$$

and with the substitution of $RT=c_s^2=c^2/3$ (or $\|\sqrt{2RT}\zeta_1\|=\sqrt{3RT}=c$), we obtain the equilibrium distribution function of the 9-bit LBE model:

$$f_\alpha^{(\mathrm{eq})}=w_\alpha\rho\left\{1+\frac{3(\boldsymbol{e}_\alpha\cdot\boldsymbol{u})}{c^2}+\frac{9(\boldsymbol{e}_\alpha\cdot\boldsymbol{u})^2}{2c^4}-\frac{3\boldsymbol{u}^2}{2c^2}\right\}.\tag{40}$$

C. Three-dimensional 27-bit square lattice model

The 27-bit LBE model in 3D square lattice space is a straightforward extension of the 2D 9-bit model. The abscissas ξ_i, as well as the corresponding weight coefficients ω_i, of the quadrature to evaluate the moments remain the same. Therefore,

$$I=\frac{\rho}{\pi^{3/2}}\sum_{i,j,k=1}^{3}\omega_i\omega_j\omega_k\psi(\boldsymbol{\xi}_{i,j,k})\times\left\{1+\frac{(\boldsymbol{\xi}_{i,j,k}\cdot\boldsymbol{u})}{RT}+\frac{(\boldsymbol{\xi}_{i,j,k}\cdot\boldsymbol{u})^2}{2(RT)^2}-\frac{\boldsymbol{u}^2}{2RT}\right\},\tag{41}$$

where $\boldsymbol{\xi}_{i,j,k}=(\xi_i,\xi_j,\xi_k)=\sqrt{2RT}(\zeta_i,\zeta_j,\zeta_k)$. With the following notations similar to the 9-bit model,

$$\boldsymbol{e}_\alpha=\begin{cases}(0,0,0), & \alpha=0\\ (\pm1,0,0)c,\ (0,\pm1,0)c,\ (0,0,\pm1)c, & \alpha=1,2,...,6\\ (\pm1,\pm1,0)c,\ (\pm1,0,\pm1)c,\ (0,\pm1,\pm1)c, & \alpha=7,8,...,18\\ (\pm1,\pm1,\pm1)c, & \alpha=19,20,...,26\end{cases}\tag{42}$$

and

$$w_\alpha=\frac{\omega_i\omega_j\omega_k}{\pi^{3/2}}=\begin{cases}8/27, & i=j=k=2, & \alpha=0\\ 2/27, & i=j=2,\ k=1,\ \ldots, & \alpha=1,2,...,6\\ 1/54, & i=j=1,\ k=2,\ \ldots, & \alpha=7,8,...,18\\ 1/216, & i=j=k=1,\ \ldots, & \alpha=19,20,...,26,\end{cases}\tag{43}$$

we obtain the equilibrium distribution function of the 27-bit LBE model:

$$f_\alpha^{(\mathrm{eq})}=w_\alpha\rho\left\{1+\frac{3(\boldsymbol{e}_\alpha\cdot\boldsymbol{u})}{c^2}+\frac{9(\boldsymbol{e}_\alpha\cdot\boldsymbol{u})^2}{2c^4}-\frac{3\boldsymbol{u}^2}{2c^2}\right\}.\tag{44}$$

Note that the $f_\alpha^{(\mathrm{eq})}$ of the 27-bit model is exactly the same as that of the 9-bit model except for the values of the coefficients w_α. Also, the sound speed of the 27-bit model is identical to that of the 9-bit model because in both models $RT=c_s^2=c^2/3$.

V. CONCLUSION

Recently, a number of gas kinetic methods have been developed for solving Navier-Stokes equations of simple and complex fluids [27–33]. All these methods are based upon the solution of the BGK equation (1). In particular, these gas kinetic methods are basically a finite-volume solution of Eq. (8) and they do not require discretization of the velocity space $\boldsymbol{\xi}$. While the lattice Boltzmann equation is in the incompressible limit due to the small-Mach-number expansion, the gas kinetic methods are particularly suitable for shock capture.

In conclusion, we have derived lattice Boltzmann models from the Boltzmann BGK equation, which is completely independent of lattice-gas automata. The derivation directly connects the lattice Boltzmann equation to the Boltzmann equation; thus, the framework of the lattice Boltzmann equation can rest on that of the Boltzmann equation and the rigorous results of the Boltzmann equation can be extended to the lattice Boltzmann equation via this explicit connection. Insight to improve the previous LBE models can also be gained from the results obtained in this paper [24–26]. Furthermore, the analysis here also points out the relationship between the LBE method and other newly developed gas kinetic methods [27–33].

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