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SEMICLASSICAL LATTICE BOLTZMANN EQUATION HYDRODYNAMICS

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Abstract

A semiclassical lattice Boltzmann method has been recently developed based on projecting the Uehling-Uhlenbeck Boltzmann BGK equation onto the tensor Hermite polynomials (Phys. Rev. E, 79 012345). Both the non-eqilibrium and equilibrium distribution functions are expanded to the same order. The intrinsic discrete nodes of the Gauss-Hermite quadrature provide the natural lattice velocities for the semicalssical lattice method. Lattice Boltzmann methods for two-dimensional and axisymmetric flows are presented. The approach of Halliday et al (Phys. Rev. E 64 011208) is adopted to derive the axisymmetric LBM. The Chapman-Enskog multiscale analysis of the methods are also given. Gases of particles of Bose-Einstein and Fermi-Dirac statistics are considered and the classical Maxwell-Boltzmann statistics can be recovered in the classical limit. Simulations of flows over a circular cylinder and a sphere are included to illustrate the present methods.

KEYWORDS: Uehling-Uhlenbeck Boltzmann equation, Semiclassical lattice Boltzmann method, Quantum statistics, Quantum hydrodynamics.

I. INTRODUCTION

Lattice Boltzmann method (LBM) is based on the kinetic equations for simulating fluid flow, see [1,2]. The LBM originated from its predecessor, the lattice gas cellular automata (LGCA) models [3]. Over the past two decades, significant advances in the development of the lattice Boltzmann methods [4-7] based on classical Boltzmann equations with the relaxation time approximation of Bhatnagar, Gross and Krook (BGK) [8] have been achieved. The lattice Boltzmann methods have demonstrated its ability to simulate hydrodynamic systems, magnetohydrodynamic systems, multi-phase and multi-component fluids, multi-component flow through porous media, and complex fluid systems, see Ref. [9]. Most of the classical LBMs are accurate up to the second order, i.e., Navier-Stokes hydrodynamics and have not been extended beyond the level of the Navier-Stokes hydrodynamics. A systematical method [10,11] was proposed for kinetic theory representation of hydrodynamics beyond the Navier-Stokes equations using Grad's moment expansion method [12]. The use of Grad's moment expansion method in other kinetic equations such as quantum kinetic equations and Enskog equations can be found in Refs. [13,14].

Despite their great success, however, most of the existing lattice Boltzmann methods are limited to hydrodynamics of classical particles. Modern development in nanoscale transport requires carriers of particles of arbitrary statistics, e.g., phonon Boltzmann transport in nanocomposite and carrier transport in semiconductors. The extension and generalization of the successful classical LBM to quantum lattice Boltzmann method for quantum particles is desirable. Analogous to the classical Boltzmann equations, a semiclassical Boltzmann equations for transport phenomenon in quantum gases has been developed by Uehling and Uhlenbeck (UUB)[15]. Following the work of Uehling and Uhlenbeck based on the Chapman-Enskog procedure [16], the hydrodynamic equations of a trapped dilute Bose gas with damping have been derived [17]. In [13], the quantum Grad expansion using tensor Hermite polynomials has been applied to obtain the non-equilibrium density matrix which reduces to the classical Grad moment expansion if the gas obeys the Boltzmann statistics. The full Boltzmann equations is mathematically difficult to handle due to the collision integral in different types of collisions. Also, BGK-type relaxation time models to capture the essential properties of carrier scattering mechanisms can be similarly devised for the Uehling-Uhlenbeck Boltzmann equations for various carriers and have been widely used in carrier transports [17]. Recently, kinetic numerical methods for ideal quantum gas dynamics based on Bose-Einstein and Fermi-Dirac statistics have been presented [18,19]. A gas-kinetic method for the semiclassical Boltzmann-BGK equations for non-equilibrium transport has been devised [20]. A newly developed semiclassical lattice Boltzmann method has been presented [21].

In this work, we derive and analyze a class of new semiclassical lattice Boltzmann method for the Uehling-Uhlenbeck Boltzmann-BGK (UUB-BGK) equations based on Grad's moment expansion method. Axisymmetric semiclassical LBM is also considered by adopting the method of Halliday et al. [22] and Zhou [23]. We also apply the Chapman-

Enskog method [16] to the UUB-BGK equations to obtain the relations between the relaxation time and viscosity and thermal conductivity which provide the basis for determining relaxation time used in the present semiclassical LBM. Hydrodynamics based on moments up to second and third order expansions are presented. Computational examples to illustrate the methods are given and the effects due to quantum statistics are delineated.

II. BASIC THEORY

We consider the Uehling-Uhlenbeck Boltzmann-BGK equations

$$\frac{\partial f}{\partial t} + \frac{\vec{p}}{m} \cdot \nabla_{\vec{x}} f = -\frac{(f - f^{(0)})}{\tau}, \tag{1}$$

where m is the particle mass, $f(\vec{p}, \vec{x}, t)$ is the distribution function which represents the average density of particles with momentum $\vec{p}$ at the space-time point $\vec{x}, t$. In (1), τ is the relaxation time which is in general dependent on the macroscopic variables and $f^{(0)}$ is the local equilibrium distribution given by

$$f^{(0)} = \{\exp[\frac{(\vec{p} - m\vec{u})^2}{2mk_BT} - \frac{\mu}{k_BT}] - \theta\}^{-1}, \tag{2}$$

where $\vec{u}$ is the mean macroscopic velocity, T is the temperature, μ is the chemical potential, k_B is the Boltzmann constant and $\theta = -1$ denotes the Fermi-Dirac (FD) statistics, $\theta = +1$ the Bose-Einstein (BE) statistics and $\theta = 0$, the Maxwell-Boltzmann (MB) statistics. Once the distribution function is known, the macroscopic quantities, the number density, number density flux, and energy density are defined, respectively, by

$$\Phi(\vec{x}, t) = \int \frac{d\vec{p}}{h^3} \phi f, \tag{3}$$

where $\Phi = (n, n\vec{u}, \epsilon, P_{\alpha\beta}, Q_\alpha)^T$ and $\phi = (1, \vec{\xi}, \frac{m}{2}c^2, c_\alpha c_\beta, \frac{m}{2}c^2 c_\alpha)^T$. Here, $\vec{\xi} = \vec{p}/m$ is the particle velocity and $\vec{c} = \vec{\xi} - \vec{u}$ is the thermal velocity. The gas pressure is defined by $P(\vec{x}, t) = P_{\alpha\alpha}/3 = 2\epsilon/3$. Just as in the classical case one can derive from Eq. (1) a set of general transport equations. Multiplying Eq. (1) by $1, \vec{p}$, or $\vec{p}^2/2m$, and integrating the resulting equations over all $\vec{p}$, then one can obtain the general hydrodynamical equations.

III. EXPANSION OF DISTRIBUTION FUNCTION USING GRAD'S METHOD

To derive the lattice UUB-BGK method, we look for approximate solution to the UUB-BGK equation and meanwhile keep the representation in a kinetic theory setting. It is emphasized that as a partial sum of Hermite series with finite terms, the truncated distribution function f^N can be completely and uniquely determined by its values at a set of discrete abscissae in the velocity space. This is possible because with f truncated to order N, we have:

$$f^N(\vec{x}, \vec{\zeta}, t)\mathcal{H}^{(n)}(\vec{\zeta}) = \omega(\vec{\zeta})q(\vec{x}, \vec{\zeta}, t) \tag{4}$$

where $q(\vec{x}, \vec{\zeta}, t)$ is a polynomial in ζ of a degree no greater than $2N$. Using the Gauss-Hermite quadrature, $\mathbf{a^{(n)}}$ can be precisely calculated as a weighted sum of functional values of $q(\vec{x}, \vec{\zeta}, t)$:

$$\mathbf{a}^{(n)}(\vec{x}, t) = \int_{-\infty}^{\infty} \omega(\vec{\zeta})q(\vec{x}, \vec{\zeta}, t)d\vec{\zeta} = \sum_{1}^{l} w_a q(\vec{x}, \vec{\zeta}_a, t) = \sum_{1}^{l} \frac{w_a}{\omega(\vec{\zeta}_a)} f^N(\vec{x}, \vec{\zeta}_a, t)\mathcal{H}^{(n)}(\vec{\zeta}_a), \tag{5}$$

where w_a and $\vec{\zeta}_a, a = 1, ..., l$, are, respectively, the weights and abscissae of a Gauss-Hermite quadrature of degree $\geq 2N$. Thus, f^N is completely determined by the set of discrete functional values, $f^N(\vec{x}, \vec{\zeta}_a, t); a = 1, ..., l$, and therefore its first N velocity moments, and vise versa. The set of discrete distribution functions $f^N(\vec{x}, \vec{\zeta}_a, t)$ now serve as a new set of fundamental variables (in physical space) for defining the fluid system in place of the conventional hydrodynamic variables.

Next, we expand the equilibrium distribution $f^{(0)}$ in the Hermite polynomial basis to the same order as f^N, i.e., $f^{(0)}(\vec{x}, \vec{\zeta}, t) \approx f^{(0)N}(\vec{x}, \vec{\zeta}, t)$, and we have

$$f^{(0)N}(\vec{x}, \vec{\zeta}, t) = \omega(\vec{\zeta}) \sum_{n=0}^{N} \frac{1}{n!} \mathbf{a}_0^{(n)}(\vec{x}, t) \cdot \mathcal{H}^{(n)}(\vec{\zeta}) \tag{6}$$

$$\mathbf{a}_0^{(n)}(\vec{x}, t) = \int f^{(0)}(\vec{x}, \vec{\zeta}, t)\mathcal{H}^{(n)} d\vec{\zeta} \tag{7}$$

These coefficients $\mathbf{a}_0^{(n)}$ can be evaluated exactly and we have

$$\mathbf{a}_0^{(0)} = n = T^{3/2} g_{3/2}(z),\ \mathbf{a}_0^{(1)} = n\vec{u}, \mathbf{a}_0^{(2)} = n[\vec{u}\vec{u} + (T\frac{g_{5/2}(z)}{g_{3/2}(z)} - 1)\delta], \mathbf{a}_0^{(3)} = n[\vec{u}\vec{u}\vec{u} + (T\frac{g_{5/2}(z)}{g_{3/2}(z)} - 1)\delta\vec{u}] \tag{8}$$

where n,$\vec{u}$ and T are in non-dimensional form hereinafter.

Denote $f_a^{(0)} \equiv w_a f^{(0)}(\vec{\zeta}_a)/\omega(\vec{\zeta}_a)$ and for $N = 3$, we get the explicit Hermite expansion of the Bose-Einstein (or Fermi-Dirac) distribution at the discrete velocity $\vec{\zeta}_a$ as:

$$f_a^{(0)} = w_a n\{1 + \vec{\zeta}_a \cdot \vec{u} + \frac{1}{2}[(\vec{u}\cdot\vec{\zeta}_a)^2 - u^2 + (T\frac{g_{5/2}(z)}{g_{3/2}(z)} - 1)(\zeta_a^2 - D)] + \frac{\vec{\zeta}\cdot\vec{u}}{6}[(\vec{u}\cdot\vec{\zeta}_a)^2 \\ -3u^2 + 3(T\frac{g_{5/2}(z)}{g_{3/2}(z)} - 1)(\zeta_a^2 - D - 2)]\}. \tag{9}$$

where $D = \delta_{ii}$.

We note that the above development follows closely the works presented in [12,13] for the classical statistics. We also note that for the case of Maxwell-Boltzmann statistics, $\theta = 0$, the $\mathbf{a}_0^{(n)}$ and $f_a^{(0)}$ are of the same form as Eq. (8) and Eq. (9) except that all the $g_\nu(z)$ in them are set equal to z. Thus, we can recover the classical counterpart [12].

IV. A SEMICLASSICAL LATTICE BOLTZMANN-BGK METHOD

Once we have obtained f^N and $f^{(0)N}$ at the discrete velocity abscissae $\vec{\zeta}_a$, we are ready to derive the governing equations for $f^N(\vec{\zeta}_a)$ in the physical configuration space. We have the set of governing equations for $f_a, a = 1, ..., l$, as

$$\frac{\partial f_a(\vec{x},t)}{\partial t} + \vec{\zeta}_a \cdot \nabla_{\vec{x}} f_a(\vec{x},t) = -\frac{(f_a(\vec{x},t) - f_a^{(0)})}{\tau}, \tag{10}$$

where $f_a^{(0)}$ is given by Eq. (9) and τ will be specified below. Applying Gauss-Hermite quadrature to the moment integration, we have the macroscopic quantities, the number density, number density flux, and energy density. And the macroscopic variables become:

$$n(\vec{x},t) = \sum_{a=1}^{l} f_a(\vec{x},t),\ n\vec{u} = \sum_{a=1}^{l} f_a\vec{\zeta}_a,\ n(DT\frac{g_{5/2}(z)}{g_{3/2}(z)} + u^2) = \sum_{a=1}^{l} f_a\zeta_a^2. \tag{11}$$

In summary, equations (10) and (9) form a closed set of differential equations governing the set of variables $f_a(\vec{x},t)$ in the physical configuration space. All the macroscopic variables and their fluxes can be calculated directly from their corresponding moment summations.

We discretize Eq. (10) in configuration space $(\vec{x},t)$ by employing first-order upwind finite-difference approximation for the time derivative on the left-hand side and choose the time step $\triangle t = 1$, we then have the following standard form of the lattice UUB-BGK method:

$$f_a(\vec{x} + \vec{\zeta}_a, t+1) - f_a(\vec{x},t) = -\frac{1}{\tau}[f_a - f_a^{(0)}]. \tag{12}$$

The selection of $\vec{\zeta}_a$ is made to maximize the algebraic degree of precision for the given number of abscissae l. Here, standard 1D5Q and 2D9Q lattices and their corresponding weights can be employed. Lastly, it is necessary to specify a value for each lattice at the boundaries when fluid flow is simulated with lattice Boltzmann methods. An interesting presentation of boundary conditions in a rarefied quantum gas has been given [25]. Most traditional boundary condition methods of classical LBM can be applied here.

V. RESULTS AND DISCUSSION

In this section, we report some numerical examples to test the theory and to illustrate the present semiclassical lattice Boltzmann method. For validation and comparison purposes, We consider a uniform two-dimensional viscous flow over a circular cylinder in a quantum gas to illustrate the present semiclassical lattice Boltzmann method in

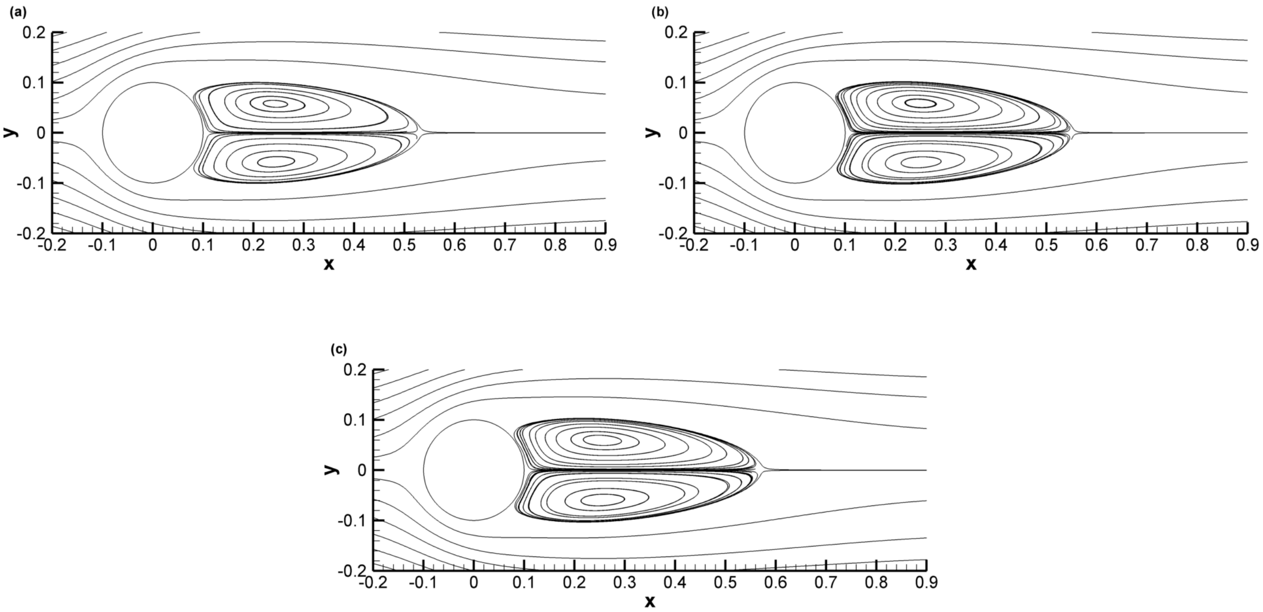

FIG. 1: Streamlines of uniform flow over a circular cylinder in a quantum gas with $z = 0.2$ and $Re_\infty = 40$. (a) BE gas, (b) MB gas, (c) FD gas.

practical flow simulation. We used the $N = 2$ expansion equations set for this case. The computation domain is $(-1, 1) \times (-1, 1)$ and set by 201×201 lattices, and the cylinder is set at the center of the computation domain with the radius $D = 0.1$. Uniform Cartesian grid system is used. The free stream velocity is $U_\infty = 0.1$, free stream temperature $T_\infty = 0.5$ and the Reynolds number $Re_\infty = U_\infty D/\nu$. We consider two cases with $Re_\infty = 20$ and $Re_\infty = 40$. The kinetic viscosity ν of the fluid could be obtained from the given Reynolds number and the relaxation time τ is calculated according to $\tau_q = \frac{\nu}{T}\frac{g_{3/2}(z)}{g_{5/2}(z)} + \frac{\delta t}{2}$, rather than the classical one $\tau_c = \frac{\nu}{T} + \frac{\delta t}{2}$, and both of them come from Chapman-Enskog analysis which considers the numerical viscosity in lattice Boltzmann scheme. The equilibrium density distribution function with the given free stream velocity and density is used to implement the boundary conditions at the far fields and at the cylinder surface. A better boundary treatment using the immersed boundary velocity correction method proposed in [25] which accurately enforcing the physical boundary condition is also adopted here. The standard D2Q9 velocity lattice was used. The results for the case $Re_\infty = 40$ are shown in Fig. 1. The flow patterns are symmetric and the vortices in the wake region become larger as compared with $Re_\infty = 20$ case. The size of the vortex for the MB gas is always larger than that of BE gas and smaller than that of FD gas. This reflects the fact that the Maxwell-Boltzmann distribution always lies in between the Bose-Einstein and Fermi-Dirac distributions. Theoretically, as comparing with particles of classical statistics, the effects of quantum statistics at finite temperatures (non-degenerate case) are approximately equivalent to introducing an interaction between particles [26]. This interaction is attractive for bosons and repulsive for fermions and operates over distances of order of the thermal wavelength Λ. Our present simulation examples seem to be able to illustrate and explore the manifestation of the effect of quantum statistics.

Next, We consider another case, a uniform two-dimensional pressure-driven channel flow in a quantum gas. The channel length is L and height H and $L/H = 25$. With the given fugacity $z_{inlet} = 0.2$,$z_{outlet} = 0.0983503$ for the Fermi gas, $z_{inlet} = 0.2$,$z_{outlet} = 0.101913$ for the Bose gas, and $z_{inlet} = 0.2$,$z_{outlet} = 0.1$ for the classical limit, the temperature is $T_{inlet} = 0.5$,$T_{outlet} = 0.5$,then the pressure ratio will be $(P_{inlet}/P_{outlet}) = (nT\frac{g_{\frac{5}{2}}(z)}{g_{\frac{3}{2}}(z)})_{inlet}/(nT\frac{g_{\frac{5}{2}}(z)}{g_{\frac{3}{2}}(z)})_{outlet} = g_{\frac{5}{2}}(z_{inlet})/g_{\frac{5}{2}}(z_{outlet}) = 2$ for the three cases. Since the D2Q9 square lattice is applied, L can be written as $L = (N_x - 1)\delta_x$, and $H = (N_y - 1)\delta_y$ where N_x and N_y are the number of lattice nodes in the x- and y-direction, respectively. To begin with the computation, the desired $Kn = \lambda/H$ is first input, where H is the height of the channel. We also set the lattice spacing $\delta_x = \delta_y = 1$. The relaxation time τ can be expressed as $\tau = Kn(N_y - 1)$. Having Kn defined, appropriate N_y and τ could be chosen, which could then be used in the determination of mesh size and the collision propagation updating procedure, respectively. We used the $N = 2$ expansion equations set for all the cases computed. The computation domain is $(0 \leq x \leq 500, 0 \leq y \leq 20)$ and 501×21 uniform lattices were

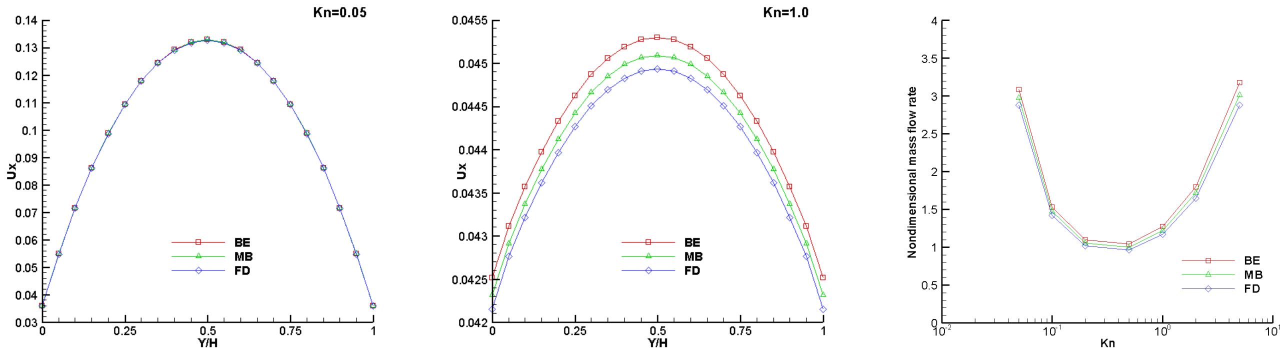

FIG. 2: Velocity profiles in a channel flow of gases of arbitrary statistics (gas with $z = 0.2$). (a) Kn=0.05, (b) Kn=1, (c) mass flow rate.

used. Several Knudsen numbers covering near continuum, slip and transition flow regimes are calculated.

The steady velocity profiles for the three statistics, BE, MB, and FD gases for the case of $z = 0.2$ are shown in Fig. 2, respectively, for three different Knudsen numbers to represent the Knudsen, slip and Poiseuille regions. For the small Knudsen number, $Kn = 0.05$, the characteristic parabolic velocity profile is evident and for $Kn = 1.0$, the velocity slip at the walls can be clearly observed. Again, the profile for MB gas lies always in between that of the BE and FD gas and for small Knudsen number, the three profiles get closer to each other.

VI. CONCLUDING REMARKS

To conclude, a new lattice Uehling-Uhlenbeck Boltzmann-BGK method is derived for dilute quantum gas hydrodynamics and beyond. The method is obtained by first projecting the UUB-BGK equations onto the Hermite polynomial basis as pioneered by Grad. The equilibrium distribution of lattice Boltzmann equations for simulating fully compressible flows is derived through expanding Bose-Einstein (or Fermi-Dirac) distribution function onto Hermite polynomial basis which is done in *a priori* manner and is free of usual *ad hoc* parameter-matching. Second, finite order expansions up to third order are considered and compared with traditional classical lattice Boltzmann-BGK methods. The present work can be considered as an extension and generalization of the work of Shan and He [10] for quantum gas and share equally many desirable properties claimed by them, such as free of drawbacks in conventional higher-order hydrodynamic formulations. Moreover, our development recovers their classical results when the classical limit is taken. The hydrodynamics beyond the semiclassical Navier-Stokes equations can also be explored if higher than third order expansion is taken. The present construction provides quantum Navier-Stokes order solution and beyond. Several computational examples of both Bose-Einstein and Fermi-Dirac gases in one dimensional shock tube flow and two dimensional flows over circular cylinder have been simulated and the results are very encouraging and exhibit similar flow characteristics of their corresponding classical cases. The effect of quantum statistics on the hydrodynamics is clearly delineated. The experimental results for quantum hydrodynamics are rare and we only validate our results with the corresponding classical counterpart. The external potential term can be added to the UUB-BGK equations to treat external force or other interaction potential for more complex systems. Lastly, the present development of semiclassical lattice Boltzmann method provides a unified framework for a parallel treatment of gas systems of particles of arbitrary statistics.

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