Lattice Uehling-Uhlenbeck Boltzmann-Bhatnagar-Gross-Krook hydrodynamics of quantum gases

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We present a semiclassical lattice Boltzmann method based on quantum kinetic theory. The method is directly derived by projecting the Uehling-Uhlenbeck Boltzmann-Bhatnagar-Gross-Krook equations onto the tensor Hermite polynomials following Grad's moment expansion method. The intrinsic discrete nodes of the Gauss-Hermite quadrature provide the natural lattice velocities for the semiclassical lattice Boltzmann method. Gases of particles of arbitrary statistics can be considered. Simulation of one-dimensional compressible gas flow and two-dimensional hydrodynamic flows are shown. The results indicate distinct characteristics of the effects of quantum statistics.

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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, multiphase and multicomponent fluids, multicomponent flow through porous media, and complex fluid systems, see [9]. The lattice Boltzmann equations (LBEs) can also be directly derived in *a priori* manner from the continuous Boltzmann equations [10,11]. 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 [12,13] was proposed for kinetic theory representation of hydrodynamics beyond the Navier-Stokes equations using Grad's moment expansion method [14]. The use of Grad's moment expansion method in other kinetic equations such as quantum kinetic equations and Enskog equations can be found in [15,16].

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 equation for transport phenomenon in quantum gases has been developed by Uehling and Uhlenbeck (UUB) [17]. Following the work of Uehling and Uhlenbeck based on the Chapman-Enskog procedure [18], the hydrodynamic equations of a trapped dilute Bose gas with damping have been derived [19]. In [15], the quantum Grad expansion using tensor Hermite polynomials has been applied to obtain the nonequilibrium 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. To avoid the complexity of the collision term, the relaxation-time model originally proposed by BGK [8] for the classical nonrelativistic neutral and charged gases has been widely used. 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 [20]. Recently, kinetic numerical methods for ideal quantum gas dynamics based on Bose-Einstein and Fermi-Dirac statistics have been presented [21,22]. A gas-kinetic method for the semiclassical Boltzmann-BGK equations for nonequilibrium transport has been devised [23]. It is noted that the approaches presented in [21–23] are based on the semiclassical kinetic description, i.e., the particle motion (velocity or momentum) and position are treated in classical mechanics manner while the particles can be of quantum statistics. We also emphasize that several quantum lattice-gas cellular automata methods [24–28] have been recently presented which are applying and extending the concept of classical LGCA models to treat the time evolution of wave functions for spinning particles and the Schrödinger equation or the Dirac equation directly. For a more detailed review, see [29].

In this work, we derive a different semiclassical lattice Boltzmann method for the Uehling-Uhlenbeck Boltzmann-BGK (UUB-BGK) equations based on Grad's moment expansion method by projecting the UUB-BGK equations onto Hermite polynomial basis. We also apply the Chapman-Enskog method [18] to the UUB-BGK equations to obtain the relations between the relaxation time, 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 illustrating the methods are given and the effects due to quantum statistics are delineated.

This paper is organized as follows. Section II gives a brief description of basic semiclassical kinetic theory. The projection of Uehling-Uhlenbeck Boltzmann-BGK equations onto

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the Hermite polynomials is derived in Sec. III. The lattice Boltzmann equations for quantum gases is given in Sec. IV. Some computational examples and discussion of results are given in Sec. V. Concluding remarks are given in Sec. VI.

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 and $f(\vec{p},\vec{x},t)$ is the distribution function which represents the average density of particles with momentum $\vec{p}$ at the space-time point $\vec{x}$, t. In Eq. (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

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

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 $\phi=(1,\vec{\xi},\frac{m}{2}c^2,c_\alpha c_\beta,\frac{m}{2}c^2c_\alpha)^T$. 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 obtains the general hydrodynamical equations

$$\frac{\partial n}{\partial t}+\nabla_{\vec{x}}\cdot(n\vec{u})=0, \tag{4}$$

$$n\left(\frac{\partial}{\partial t}+\vec{u}\cdot\nabla_{\vec{x}}\right)u_\alpha+\frac{\partial P_{\alpha\beta}}{\partial x_\beta}=0, \tag{5}$$

$$\frac{\partial\epsilon}{\partial t}+\nabla_{\vec{x}}\cdot(\epsilon\vec{u})+\nabla_{\vec{x}}\cdot\vec{Q}+D_{\alpha\beta}P_{\alpha\beta}=0, \tag{6}$$

where $D_{\alpha\beta}=(\partial u_\alpha/\partial x_\beta+\partial u_\beta/\partial x_\alpha)/2$ is the rate of strain tensor.

For the zeroth order equilibrium distribution function, the hydrodynamical variables can be explicitly expressed in terms of Boson or Fermi function, see [30]. For example, the number density $n(x,t)$ is given by

$$n(\vec{x},t)=\int_{-\infty}^{\infty}\frac{d^3p}{h^3}f^{(0)}=\frac{1}{\Lambda^3}g_{3/2}[z(\vec{x},t)], \tag{7}$$

where $\Lambda=[2\pi h^2/mk_BT(\vec{x},t)]^{1/2}$ is the de Broglie thermal wavelength and h is the Planck constant. The stress tensor P_{ij}, pressure P, and heal flux vector Q_i become

$$P_{ij}=P\delta_{ij},\quad P=\frac{k_BT}{\Lambda^3}g_{5/2}(z),\quad Q_i=0. \tag{8}$$

Here $z(\vec{x},t)=e^{\mu(\vec{x},t)/k_BT}$ is the fugacity. The function g_ν represents either the Bose-Einstein or Fermi-Dirac function of order ν which is defined as

$$g_\nu(z)\equiv\frac{1}{\Gamma(\nu)}\int_0^\infty\frac{x^{\nu-1}}{z^{-1}e^x+\theta}dx=\sum_{l=1}^{\infty}(-\theta)^{l-1}\frac{z^l}{l^\nu}, \tag{9}$$

where $\Gamma(\nu)$ is the gamma function. Furthermore, the corresponding hydrodynamic equations integrated from the zeroth order solution give the "quantum Euler equations" in which the heat flux and the shear viscosity are zero in this case.

The first-order distribution function for the UUB-BGK equations according to the Chapman-Enskog procedure assumes the form [23]:

$$f^{(1)}=f^{(0)}[1+\psi(1-\theta f^{(0)})], \tag{10}$$

$$\psi=-\tau\left\{\frac{c\cdot\nabla T}{T}\left[\frac{mc^2}{2k_BT}-\frac{5g_{5/2}(z)}{2g_{3/2}(z)}\right]+\frac{m}{k_BT}\frac{\partial u_\mu}{\partial x_v}\left(c_\mu c_v-\frac{1}{3}\delta_{\mu v}c^2\right)\right\}. \tag{11}$$

The viscosity η and thermal conductivity κ for a quantum gas can be derived in terms of the relaxation time as

$$\eta=\tau nk_BT\frac{g_{5/2}(z)}{g_{3/2}(z)}, \tag{12}$$

$$\kappa=\tau\frac{5k_B}{2m}nk_BT\left[\frac{7}{2}\frac{g_{7/2}(z)}{g_{3/2}(z)}-\frac{5}{2}\frac{g_{5/2}(z)}{g_{3/2}(z)}\right]. \tag{13}$$

The relaxation times for various scattering mechanisms of different carrier transport in semiconductor devices including electrons, holes, phonons, and others have been proposed [20]. The hydrodynamic equations integrated from the first-order distribution $f^{(1)}$ give the "quantum Navier-Stokes equations."

III. EXPANSION OF DISTRIBUTION FUNCTION USING GRAD'S METHOD

In this section, following the approaches in [12–16], we adopt the Grad's moment approach and seek solutions to Eq. (1) by expanding $f(\vec{x},\vec{\zeta},t)$ in terms of Hermite polynomials,

$$f(\vec{x},\vec{\zeta},t)=\omega(\vec{\zeta})\sum_{n=0}^{\infty}\frac{1}{n!}\mathbf{a}^{(n)}(x,t)\mathcal{H}^{(n)}(\vec{\zeta}), \tag{14}$$

where $\vec{\zeta}\equiv\frac{\vec{p}}{h^3}$, $\omega(\vec{\zeta})=\frac{1}{(2\pi)^{3/2}}e^{-\vec{\zeta}^2/2}$ is the weighting function, $\mathbf{a}^{(n)}$ and $\mathcal{H}^{(n)}(\vec{\zeta})$ are rank-n tensors, and the product on the right-hand side denotes full contraction. Here and throughout the paper, the shorthand notations of Grad [14] for fully symmetric tensors have been adopted. The expansion coefficients $\mathbf{a}^{(n)}$ are given by

$$\mathbf{a}^{(n)}(\vec{x},t) = \int f(\vec{x},\vec{\zeta},t)\mathcal{H}^{(n)}(\vec{\zeta})d\vec{\zeta}. \tag{15}$$

Some of the first few tensor Hermite polynomials are given here, $\mathcal{H}^{(0)}(\vec{\zeta})=1$, $\mathcal{H}_i^{(1)}(\vec{\zeta})=\zeta_i$, $\mathcal{H}_{ij}^{(2)}(\vec{\zeta})=\zeta_i\zeta_j-\delta_{ij}$, $\mathcal{H}_{ijk}^{(3)}(\vec{\zeta})=\zeta_i\zeta_j\zeta_k-\zeta_i\delta_{jk}-\zeta_j\delta_{ik}-\zeta_k\delta_{ij}$, etc.

It is evident from Eq. (15) that all the expansion coefficients are linear combinations of the velocity moments of f. The first few expansion coefficients can be easily identified with the familiar hydrodynamic variables:

$$\mathbf{a}^{(0)} = \int f d\vec{\zeta} = n, \quad \mathbf{a}^{(1)} = \int f\vec{\zeta}d\vec{\zeta} = n\vec{u},$$

$$\mathbf{a}^{(2)} = \int f(\vec{\zeta}^2 - \delta)d\vec{\zeta} = \mathbf{p} + n(\vec{u}^2 - \delta),$$

$$\mathbf{a}^{(3)} = \int f(\vec{\zeta}^3 - \vec{\zeta}\delta)d\vec{\zeta} = \mathbf{Q} + \vec{u}(a^{(2)} - 2n\vec{u}^2), \tag{16}$$

where $d\vec{\zeta}=d\vec{p}/h^3$. The macroscopic hydrodynamic variables can also be expressed in terms of the low-order Hermite expansion coefficients,

$$n = \mathbf{a}^{(0)}, \quad n\vec{u} = \mathbf{a}^{(1)}, \quad \mathbf{P} = \mathbf{a}^{(2)} - n(\vec{u}\vec{u} - \delta),$$

$$\mathbf{Q} = \mathbf{a}^{(3)} - \vec{u}\mathbf{a}^{(2)} + 2n\vec{u}\vec{u}\vec{u}. \tag{17}$$

We also have $\epsilon=\frac{1}{2}[\mathbf{a}_{ii}^{(2)}-n(\vec{u}\vec{u}-3)]$. It is evident that the five fundamental hydrodynamic variables, ρ, $\vec{u}$, and T, and the momentum flux tensor $\mathbf{P}$ can be completely determined by the first three Hermite expansion coefficients along them, while the third order moment, the heat flux vector $\mathbf{Q}$, is completely determined by the fourth coefficient.

The orthogonality of Hermite polynomials implies that the leading moments of a distribution function up to the Nth order are preserved by truncations of the higher-order terms in its Hermite expansion. Thus, a distribution function of the UUB-BGK equation can be approximated by its projection onto a Hilbert space spanned by the first N Hermite polynomials without affecting the first N moments. Here, up to Nth order, $f^N(\vec{x},\vec{\zeta},t)$ has exactly the same velocity moments as the original $f(\vec{x},\vec{\zeta},t)$. This guaranties that a quantum gas dynamic system can be constructed by a finite set of macroscopic variables.

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 abscissas in the velocity space. This is possible because, with f truncated to order N, the integrand on the right-hand side of Eq. (15) can be expressed as

$$f^N(\vec{x},\vec{\zeta},t)\mathcal{H}^{(n)}(\vec{\zeta}) = \omega(\vec{\zeta})q(\vec{x},\vec{\zeta},t), \tag{18}$$

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

$$\begin{aligned}\mathbf{a}^{(n)}(\vec{x},t) &= \int_{-\infty}^{\infty} \omega(\vec{\zeta})q(\vec{x},\vec{\zeta},t)d\vec{\zeta} = \sum_1^l w_a q(\vec{x},\vec{\zeta}_a,t)\\ &= \sum_1^l \frac{w_a}{\omega(\vec{\zeta}_a)} f^N(\vec{x},\vec{\zeta}_a,t)\mathcal{H}^{(n)}(\vec{\zeta}_a),\end{aligned} \tag{19}$$

where w_a and $\vec{\zeta}_a, a=1,\ldots,l$, are, respectively, the weights and abscissas of a Gauss-Hermite quadrature of degree $\geq 2N$. Thus, f^N is completely determined by the set of discrete functional values, $f^N(\vec{x},\vec{\zeta}_a,t)$; $a=1,\ldots,l$, and therefore its first N velocity moments, and vice 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

$$f^{(0)N}(\vec{x},\vec{\zeta},t) = \omega(\vec{\zeta})\sum_{n=0}^{N} \frac{1}{n!}\mathbf{a}_0^{(n)}(\vec{x},t) \cdot \mathcal{H}^{(n)}(\vec{\zeta}), \tag{20}$$

$$\mathbf{a}_0^{(n)}(\vec{x},t) = \int f^{(0)}(\vec{x},\vec{\zeta},t)\mathcal{H}^{(n)}d\vec{\zeta}. \tag{21}$$

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

$$\mathbf{a}_0^{(0)} = n = T^{3/2}g_{3/2}(z), \quad \mathbf{a}_0^{(1)} = n\vec{u},$$

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

$$\mathbf{a}_0^{(3)} = n\left[\vec{u}\vec{u}\vec{u} + \left(T\frac{g_{5/2}(z)}{g_{3/2}(z)} - 1\right)\delta\vec{u}\right], \tag{22}$$

where n, $\vec{u}$, and T are in nondimensional 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

$$f_a^{(0)} = w_a n \left\{ 1 + \vec{\zeta}_a \cdot \vec{u} + \frac{1}{2}\left[(\vec{u}\cdot\vec{\zeta}_a)^2 - u^2 + \left(T\frac{g_{5/2}(z)}{g_{3/2}(z)} - 1 \right)(\zeta_a^2 - D) \right] + \frac{\vec{\zeta}\cdot\vec{u}}{6}\left[(\vec{u}\cdot\vec{\zeta}_a)^2 - 3u^2 + 3\left(T\frac{g_{5/2}(z)}{g_{3/2}(z)} - 1 \right)(\zeta_a^2 - D - 2) \right] \right\}, \tag{23}$$

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 Eqs. (22) and (23) except that all the $g_\nu(z)$ in them are set equal to z. Thus, we can recover the classical counterpart [12].

IV. SEMICLASSICAL LATTICE BOLTZMANN-BGK METHOD

Once we have obtained f^N and $f^{(0)N}$ at the discrete velocity abscissas $\vec{\zeta}_a$, 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 $f_a, a=1,\ldots,l$, as

$$\frac{\partial f_a(\vec{x},t)}{\partial t} + \vec{\zeta}_a \cdot \nabla_{\vec{x}} f_a(\vec{x},t) = -\frac{[f_a(\vec{x},t) - f_a^{(0)}]}{\tau}, \tag{24}$$

where $f_a^{(0)}$ is given by Eq. (23) and τ by Eq. (12). Applying Gauss-Hermite quadrature to the moment integration, we have the macroscopic quantities, the number density, number density flux, and energy density. Moreover the macroscopic variables become

$$n(\vec{x},t) = \sum_{a=1}^{l} f_a(\vec{x},t), \quad n\vec{u} = \sum_{a=1}^{l} f_a\vec{\zeta}_a,$$

$$n\left(DT\frac{g_{5/2}(z)}{g_{3/2}(z)} + u^2 \right) = \sum_{a=1}^{l} f_a \zeta_a^2. \tag{25}$$

In summary, Eqs. (24) and (25) 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. (24) in configuration space $(\vec{x},t)$ by employing first-order upwind finite-difference approximation for the time derivative on the left-hand side and, choosing the time step $\Delta t=1$, we then have the following standard form of the lattice UUB-BGK method:

$$f_a(\vec{x}+\vec{\zeta}_a, t+1) - f_a(\vec{x},t) = -\frac{1}{\tau}[f_a - f_a^{(0)}]. \tag{26}$$

The selection of $\vec{\zeta}_a$ is made to maximize the algebraic degree of precision for the given number of abscissas l. Here, standard D1Q5 and D2Q9 lattices and their corresponding weights can be employed. The relaxation time τ in Eq. (26) can be related to the kinematic viscosity ν through the standard Chapman-Enskog analysis of the semiclassical lattice Boltzmann method with the D2Q9 lattice model. Since the details of Chapman-Enskog analysis are well described in [31,32] and several others, here we only present the results

$$\tau_q = \frac{\nu}{T}\frac{g_{3/2}(z)}{g_{5/2}(z)} + \frac{\delta t}{2}. \tag{27}$$

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 [33]. 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 apply the numerical methods to one-dimensional quantum gas flows in a shock tube. We consider constant relaxation time $\tau=0.001$ to test the applicability of the present methods. We employ the D1Q5 discrete velocities scheme as follows:

ζ_a	w_a
0	8/15
$\pm\sqrt{5-\sqrt{10}}$	$(7+2\sqrt{10})/60$
$\pm\sqrt{5+\sqrt{10}}$	$(7-2\sqrt{10})/60$

The expansion equations up to the $N=3$ order, i.e., Eq. (23), is used for this one-dimensional problem.

The computational domain is $0\leq x\leq 1$ and is divided into uniform cells of size $1/L$, where L is the number of cells. The diaphragm is initially located at $x=0.5$. The initial conditions at the left and right sides of the diaphragm in the shock tube are $(n_l,u_l,\epsilon_l)=(1.0,0.0,1.0)$ and $(n_r,u_r,\epsilon_l)=(0.7,0.0,1.5)$. The relaxation is set to constant $\tau=0.001$. Here, we adopt the conventional finite-volume schemes as those described in [34], in which Eq. (24) is solved by first-order upwind scheme. In this case, Eq. (24) is treated as a system consisting of five one-dimensional linear wave equations. After applying first-order upwind scheme, the discrete equations become

$$\frac{f_{a,i}^{n+1} - f_{a,i}^n}{\delta t} + \zeta_a^+ \frac{f_{a,i}^n - f_{a,i-1}^n}{\delta x} + \zeta_a^- \frac{f_{a,i+1}^n - f_{a,i}^n}{\delta x} = -\frac{(f_{a,i}^n - f_{a,i}^{(0)})}{\tau}, \tag{28}$$

where $\zeta_a^+=\max(\zeta_a,0)$ and $\zeta_a^-=\min(\zeta_a,0)$, and the superscript n denotes the time level. We first performed a grid refine-

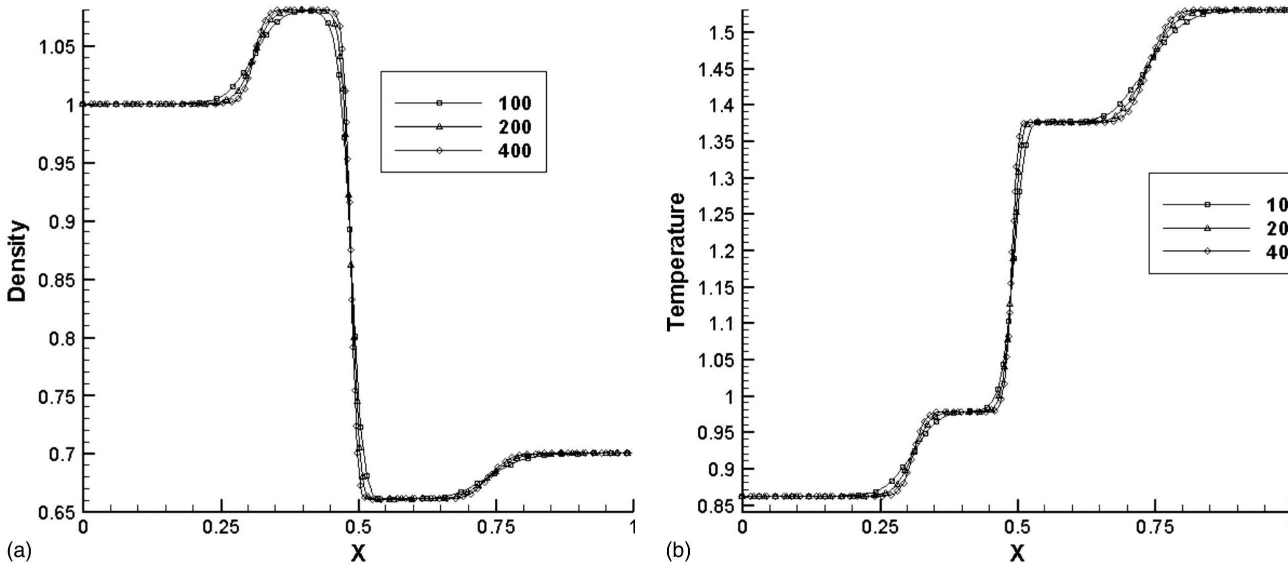

FIG. 1. Convergence of solution with refined grids. (a) Density and (b) temperature.

ment test using $L=100$, 200, and 400 cells to ensure the convergence of solution which are shown in Fig. 1. The convergence of solution is evident. Next, we compare the different behaviors due to the three statistics, namely, BE, FD, and MB statistics. The initial conditions at the left and right sides of the diaphragm in the shock tube are $(n_l,u_l,T_l)=(1.0,0.0,2.0)$ and $(n_r,u_r,T_r)=(0.7,0.0,1.8)$, and the same constant relaxation time is used. The results using $L=200$ cells for the three statistics are shown in Fig. 2. The main features of a typical shock tube flow, namely, the shock wave, contact discontinuity, and the expansion fan, are well represented. We can clearly delineate the difference of three statistics. It is shown that under different statistics although the initial temperature, density, and relaxation time are the same, the pressure, internal energy, and the temperature are different. It is noted that the results of MB statistics always lie between those of BE and FD statistics.

Next 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 practical flow simulation. We used the $N=2$ expansion equation 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 $\mathrm{Re}_\infty=U_\infty D/\nu$. We consider two cases with $\mathrm{Re}_\infty=20$ and $\mathrm{Re}_\infty=40$. The kinetic viscosity ν of the fluid could be obtained from the given Reynolds number and the relaxation time τ is calculated according to Eq. (27), rather than the classical one $\tau_c=\frac{\nu}{T}+\frac{\delta t}{2}$, and both of them come from the Chapman-Enskog analysis [31,32] 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 boundary treatment using the immersed boundary velocity correction method proposed in

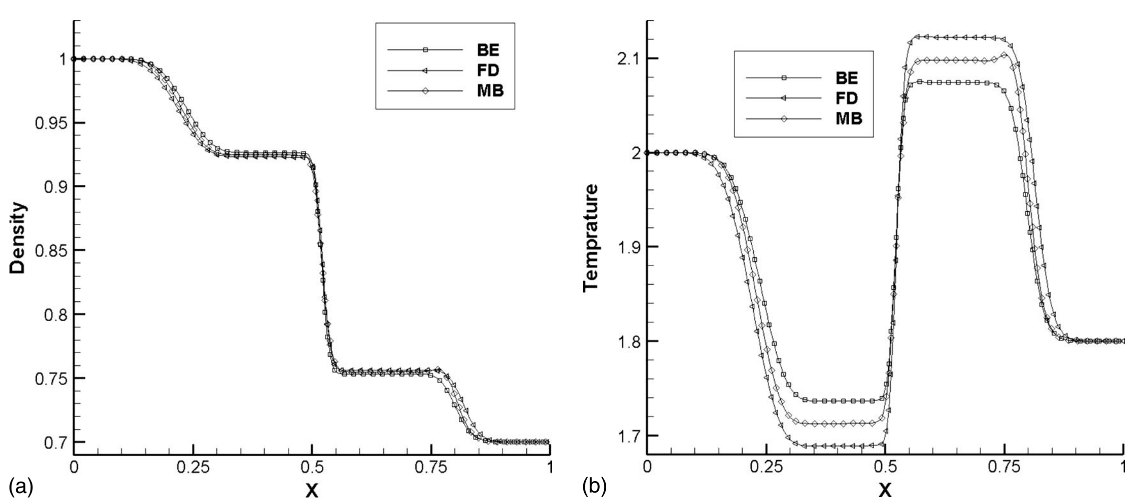

FIG. 2. Shock tube flow in a quantum gas. The effect due to different particle statistics; BE: Bose-Einstein, FD: Fermi-Dirac, MB: Maxwell-Boltzmann. (a) Density and (b) temperature.

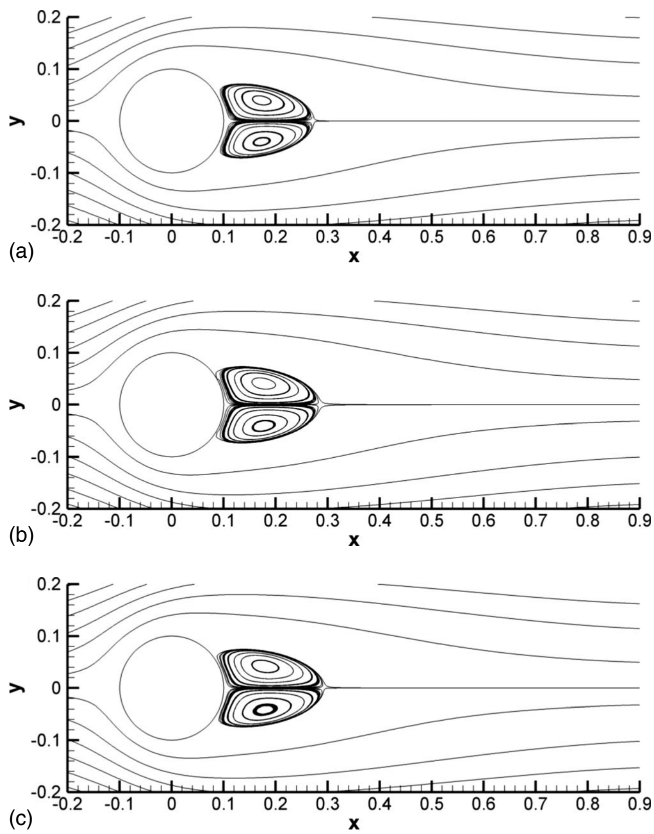

FIG. 3. Streamlines of uniform flow over a circular cylinder in a quantum gas with $z=0.2$ and $\mathrm{Re}_\infty=20$. (a) BE, (b) MB, and (c) FD gases.

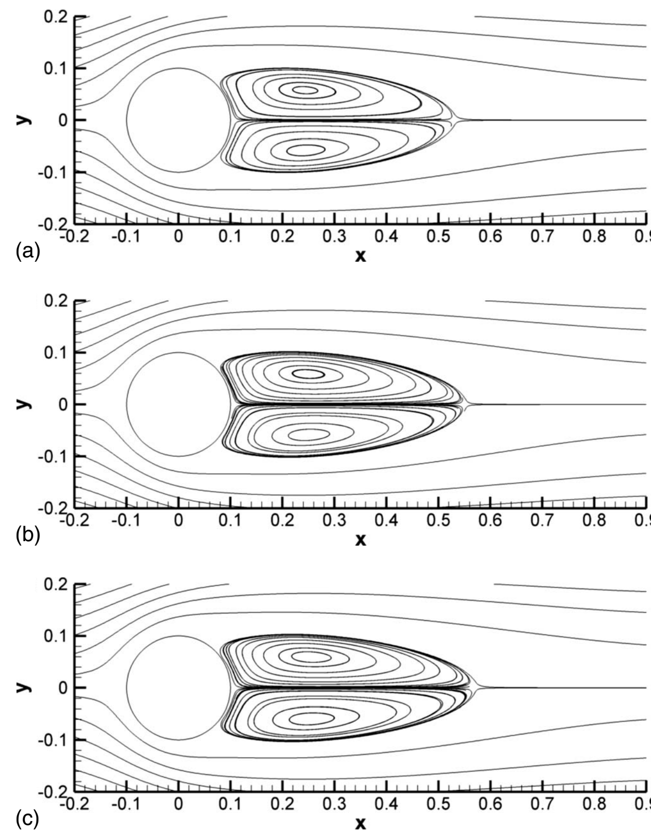

FIG. 4. Streamlines of uniform flow over a circular cylinder in a quantum gas with $z=0.2$ and $\mathrm{Re}_\infty=40$. (a) BE, (b) MB, and (c) FD gases.

[35–37], which enforces the physical boundary condition, is also adopted here. The D2Q9 velocity lattice used is as follows:

ζ_a	w_a
$(0,0)$	4/9
$(\sqrt{3},0)_{\mathrm{fs}}$	1/9
$(\pm\sqrt{3},\pm\sqrt{3})$	1/36

Here, the subscript fs denotes a fully symmetric set of points. The streamline patterns for all three statistics, BE, MB, and FD gases for the case of $\mathrm{Re}_\infty=20$ are shown in Fig. 3. For this low Reynolds number, the flow patterns are symmetric, and the wake vortices are larger for the FD gas and smaller for the BE gas as compared with the classical MB gas. Similarly, the results for the case $\mathrm{Re}_\infty=40$ are shown in Fig. 4. The flow patterns are symmetric and the vortices in the wake region become larger as compared with $\mathrm{Re}_\infty=20$ case. Again, 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 (nondegenerate case) are approximately equivalent to introducing an interaction between particles [30]. 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.

VI. CONCLUDING REMARKS

To conclude, a unique 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 [12] 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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