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Semiclassical Axisymmetric Lattice Boltzmann Method

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Abstract. A semiclassical lattice Boltzmann method is presented for axisymmetric flows of gas of particles of arbitrary statistics. The method is first derived by directly projecting the Uehling-Uhlenbeck Boltzmann-BGK equations in two-dimensional rectangular coordinates onto the tensor Hermite polynomials using moment expansion method and then the forcing strategy of Halliday et al. (Phys. Rev. E., 64 (2001), 011208) is adopted and forcing term is added into the resulting microdynamic evolution equation. The determination of the forcing terms is dictated by yielding the emergent macroscopic equations toward a particular target form. The correct macroscopic equations of the incompressible axisymmetric viscous flows are recovered through the Chapman-Enskog expansion. Computations of uniform flow over a sphere to verify the method are included. The results also indicate distinct characteristics of the effects of quantum statistics.

AMS subject classifications: 76P05, 82B40

Key words: Semiclassical lattice Boltzmann method, axisymmetric flows, flow over a sphere, Bose gas, Fermi gas.

1 Introduction

In the past two decades, significant advances have been accomplished in the development of the lattice Boltzmann methods [1–4] based on classical Boltzmann equations with the relaxation time approximation of Bhatnagar, Gross and Krook (BGK) [5]. The lattice Boltzmann method (LBM) has illustrated its capability for simulating hydrodynamic systems, magnetohydrodynamic systems, multi-phase and multi-component fluids, multi-component flow through porous media and complex fluid systems, see [6]. The lattice Boltzmann equations (LBE) can also be directly derived in *a priori* manner from the continuous Boltzmann-BGK equation [7, 8]. Most of the classical LBMs are accurate up to the second order, i.e., Navier-Stokes hydrodynamics and have

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not been extended beyond the level of the Navier-Stokes hydrodynamics. A systematical method [9,10] was proposed for kinetic representation of hydrodynamics beyond the Navier-Stokes equations using Grad's moment expansion method [11].

It is also observed that most of the existing lattice Boltzmann methods are focused on hydrodynamics of classical particles. However, modern development in nanoscale transport requires carriers of particles of arbitrary statistics [12]. The extension and generalization of the successful classical LBM to treat particles of arbitrary statistics is thus desirable. Analogous to the classical Boltzmann equation, a semiclassical Boltzmann equation which taking into account the effect of quantum statistics has been developed by Uehling and Uhlenbeck (UUB) [13]. To circumvent the mathematical difficulty of the the collision term, BGK-type relaxation time models to capture the essential properties of carrier scattering mechanisms can be similarly devised for the Uehling-Uhlenbeck Boltzmann equation for various carriers and have been widely used in carrier transport [14]. Recently, a semiclassical gas-kinetic scheme [15] has been developed for the hydrodynamic transport based on the Uehling-Uhlenbeck Boltzmann-BGK (UUB-BGK) equation. Also, a two-dimensional semiclassical lattice Boltzmann method for the UUB-BGK equation based on D2Q9 lattice model [2] and Grad's moment expansion method has been presented [16]. Hydrodynamics based on moments up to second and third order expansions are presented. Simulations of flow over a circular cylinder at low Reynolds numbers have been tested and have been found in good agreement with previous available results.

One of the most common and important classes of fluid dynamical problems is the axisymmetric flow in which flow symmetry with respect to an axis can be identified. Classical axisymmetric lattice Boltzmann method was first proposed by Halliday et al. [17] using a forcing strategy. By introducing source terms, the macroscopic equations for the axisymmetric flows can be recovered. The method of Halliday et al. has been successfully applied to a number of axisymmetric flow problems [18–26]. Recently, an interesting lattice Boltzmann model for axisymmetric flows based on Boltzmann-BGK equation in cylindrical coordinates has been proposed [27].

The main objective of this work is to present the semiclassical axisymmetric lattice Boltzmann method for axisymmetric flow of gases of arbitrary statistics. The method of Halliday et al. [17] is adopted and forcing terms are added into the two-dimensional semiclassical Boltzmann-BGK equation which are consistent in dimension with the lattice Boltzmann equation. The forcing terms are determined by demanding the emergent macroscopic equations toward a particular target form. The set of correct macroscopic equations for incompressible axisymmetric flows can be recovered through the Chapman-Enskog multiscale analysis of the semiclassical LBM.

This paper is organized as follows. Section 2 gives a brief description of element of semiclassical kinetic theory. The basic two-dimensional semiclassical lattice Uehling-Uhlenbeck Boltzmann-BGK method is described in Section 3. The derivation of the axisymmetric semiclassical LBM is given in Section 4. Simulations of uniform flow over a sphere using the present method are given in Section 5. Concluding remarks are given in Section 6.

2 Semiclassical kinetic theory

The Uehling-Uhlenbeck Boltzmann-BGK equation can be written as

$$\frac{\partial f}{\partial t}+\frac{\vec{p}}{m}\cdot\nabla_{\vec{x}}f=-\frac{\left(f-f^{(eq)}\right)}{\tau^{*}}, \tag{2.1}$$

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

$$f^{(eq)}=\left\{\exp\left[\frac{(\vec{p}-m\vec{u})^2}{2mk_BT}-\frac{\bar{\mu}}{k_BT}\right]-\theta\right\}^{-1}, \tag{2.2}$$

here $\vec{u}$ is the mean macroscopic velocity, T is the temperature, $\bar{\mu}$ 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 n, number density flux $n\vec{u}$, energy density ϵ, pressure tensor $P_{\alpha\beta}$ and heat flux vector Q_α are defined, respectively, by

$$\Phi(\vec{x},t)=\int\frac{d\vec{p}}{h^3}\phi f, \tag{2.3}$$

where

$$\Phi=(n,n\vec{u},\epsilon,P_{\alpha\beta},Q_\alpha)^T,\quad\text{and}\quad\phi=\left(1,\vec{\xi},\frac{m}{2}c^2,c_\alpha c_\beta,\frac{m}{2}c^2c_\alpha\right)^T.$$

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 $P(\vec{x},t)=P_{\alpha\alpha}/3=2\epsilon/3$. Multiplying Eq. (2.1) by $1,\vec{p}$, or $\vec{p}^2/2m$ and integrating the resulting equations over all $\vec{p}$, then one can obtain the semiclassical hydrodynamical equations. In this work, we consider the semiclassical incompressible viscous flows with rotational symmetry around the z axis. The cylindrical polar coordinates $\vec{x}=(r,\phi,z)$ system is adopted where r denoting the radial distance from axis, ϕ the azimuthal angle about axis and z the distance along axis, respectively. The mean velocity is $\vec{u}=(u_r,0,u_z)$. The governing hydrodynamic equations for the incompressible (constant n or ρ) axisymmetric viscous flows in a cylindrical polar coordinates system can be expressed as

$$\frac{\partial u_j}{\partial x_j}=-\frac{u_r}{r}, \tag{2.4a}$$

$$\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}=-\frac{1}{\rho}\frac{\partial P}{\partial x_i}+\eta\frac{\partial^2u_i}{\partial x_j^2}+\frac{\eta}{r}\frac{\partial u_i}{\partial r}-\frac{\eta u_i}{r^2}\delta_{ir}. \tag{2.4b}$$

Inserting the continuity equation into the momentum equation, we have

$$\frac{\partial u_i}{\partial t}+\frac{\partial(u_iu_j)}{\partial x_j}=-\frac{1}{\rho}\frac{\partial P}{\partial x_i}+\eta\frac{\partial^2 u_i}{\partial x_j^2}-\frac{u_iu_r}{r}+\frac{\eta}{r}\frac{\partial u_i}{\partial r}-\frac{\eta u_i}{r^2}\delta_{ir}. \tag{2.5}$$

The viscosity η for the semiclassical Boltzmann BGK model have been derived in [15] based on the Chapman-Enskog solution [28] in terms of the relaxation time as

$$\eta=\tau^* k_B T\frac{g_{\frac{5}{2}}(z)}{g_{\frac{3}{2}}(z)}. \tag{2.6}$$

Here

$$z(\vec{x},t)=e^{\bar{\mu}(\vec{x},t)/k_BT},$$

is the fugacity, the function g_ν represents for either the Bose-Einstein or Fermi-Dirac function of order ν which is defined as

$$g_\nu(z)\equiv\frac{1}{\Gamma(\nu)}\int_0^\infty\frac{x^{\nu-1}}{z^{-1}e^x+\theta}\mathrm{d}x=\sum_{l=1}^{\infty}(-\theta)^{l-1}\frac{z^l}{l^\nu}, \tag{2.7}$$

where $\Gamma(\nu)$ is the Gamma function. The relaxation times for various scattering mechanisms of different carrier transport in semiconductor devices including electrons, holes, phonons and others have been proposed [12].

The aim of this work in the following is to derive a semiclassical lattice Boltzmann equation which shall render the macroscopic continuity and momentum equations, Eqs. (2.4a) and (2.5), self-consistently.

3 Semiclassical lattice Boltzmann-BGK method

In [16], a semiclassical lattice Boltzmann method based on D2Q9 lattices in rectangular coordinates for gases of particles of arbitrary statistics has been developed. Here, for self-contained purposes, we briefly describe the essential elements of the method and use it as the basis to extend to the axisymmetric case. The Grad's moment approach was adopted to find solutions to Eq. (2.1) by expanding $f(\vec{x},\vec{\zeta},t)$ in terms of Hermite polynomials and the N-th finite order truncated distribution function f^N was considered. Since the axisymmetric equations have the two-dimensional equations embedded, here we list the essential elements of the two-dimensional semiclassical lattice Boltzmann method developed in [16]. A lattice UUB-BGK method for solving Eq. (2.1) using D2Q9 lattice model can be expressed as

$$f_a(\vec{x}+\vec{\zeta}_a\delta_t,t+\delta_t)-f_a(\vec{x},t)=-\frac{1}{\tau}\big[f_a-f_a^{(eq)}\big], \tag{3.1}$$

where $\tau = \tau^*/\delta_t$ is the dimensionless LBE relaxation time and $f_a^{(eq)}$ is the lattice equilibrium distribution function at the discrete velocity $\vec{\zeta}_a$ and for N=3, it is given by

$$
\begin{aligned}
f_a^{(eq)}(\vec{x},t) =& w_a n\Big\{1+\vec{\zeta}_a\cdot\vec{u}(\vec{x},t)+\frac{1}{2}\Big[\big(\vec{u}(\vec{x},t)\cdot\vec{\zeta}_a\big)^2-u^2(\vec{x},t)\\
&+\Big(\hat{T}(\vec{x},t)\frac{g_{5/2}(z)}{g_{3/2}(z)}-1\Big)(\zeta_a^2-D)\Big]+\frac{\vec{\zeta}_a\cdot\vec{u}}{6}\Big[(\vec{u}\cdot\vec{\zeta}_a)^2\\
&-3u^2+3\Big(\hat{T}\frac{g_{5/2}(z)}{g_{3/2}(z)}-1\Big)(\zeta_a^2-D-2)\Big]\Big\},
\end{aligned}
\tag{3.2}
$$

where $D=\delta_{ii}$ and $\hat{T}$ is the non-dimensional temperature.

The standard square $D2Q9$ lattice model is specified by

$$\vec{\zeta}_0 = (0,0), \tag{3.3a}$$

$$\vec{\zeta}_a = \Big(\cos\Big(\frac{a-1}{4}\Big)\pi, \sin\Big(\frac{a-1}{4}\Big)\Big)c, \quad a=1,\cdots,8, \tag{3.3b}$$

where $c=\delta_x/\delta_t$ is the particle streaming speed and δ_x is the lattice size and δ_t is the time step. When c is taken as 1, the lattice velocity $\vec{\zeta}_a=(\zeta_{ax},\zeta_{ay})$ has unit magnitude for directions of $a=1,3,5$ and 7 and magnitude $\sqrt{2}$ for directions of $a=2,4,6$ and 8.

Now we are ready to generalize the above two-dimensional semiclassical LBM in rectangular coordinates to axisymmetric case.

4 Semiclassical axisymmetric lattice Boltzmann method

To derive the semiclassical axisymmetric lattice Boltzmann method, we adopt the approach of Halliday et al. by incorporating a position and time dependent source or sink term into the microdynamic evolution equation as follows:

$$f_a(\vec{x}+\vec{\zeta}_a\delta_t, t+\delta_t)-f_a(\vec{x},t) = -\frac{1}{\tau}\big[f_a-f_a^{(eq)}\big]+h_a(\vec{x},t), \tag{4.1}$$

where $f_a^{(eq)}$ is given by Eq. (3.2) and $h_a(\vec{x},t)$ is an added source or sink term that will be defined later. Following the analysis of [17], we assume

$$h_a = \varepsilon h_a^{(1)}+\varepsilon^2 h_a^{(2)}+\cdots, \tag{4.2}$$

and take $h_a^{(1)}$ to be zeroth order in gradient quantities and $h_a^{(2)}$ to contain any first order gradients in macroscopic dynamic quantities $n,\vec{u}$; that is $h_a^{(n)}$ contains $(n-1)$th order gradients in n and $\vec{u}$. The issue now is to determine the $h_a^{(n)}$ that will render Eqs. (2.4a) and (2.5) in a self-consistent manner. To extract the dynamics represented by this modifying scheme, we perform the Chapman-Enskog multiscale analysis. According to the Chapman-Enskog expansion, f_a can be expressed in a series of ε

$$f_a(\vec{x}+\vec{\zeta}_a\delta_t, t+\delta_t) = \sum_0^{\infty} \frac{\varepsilon^n}{n!}(\partial_t + \vec{\zeta}_a \cdot \nabla)^n f_a, \tag{4.3a}$$

$$f_a \backsimeq f_a^{(0)} + \varepsilon f_a^{(1)} + \varepsilon^2 f_a^{(2)} + \cdots, \tag{4.3b}$$

$$\partial_t = \varepsilon\partial_{t_1} + \varepsilon^2\partial_{t_2}, \tag{4.3c}$$

$$\partial_\beta = \varepsilon\partial_{\beta_1}. \tag{4.3d}$$

The above expressions, Eqs. (4.3a)-(4.3d) are substituted into Eq. (4.1) and terms involving different orders of ε are separated as

$$f_a^{(0)} = f_a^{(eq)}, \tag{4.4a}$$

$$(\partial_{t_1} + \zeta_{a\beta}\cdot\partial_{\beta_1})f_a^{(0)} = -\frac{1}{\tau\delta_t}f_a^{(1)} + \frac{h_a^{(1)}}{\delta_t}, \tag{4.4b}$$

$$\partial_{t_2}f_a^{(0)} + \Big(1-\frac{1}{2\tau}\Big)(\partial_{t_1}+\zeta_{a\beta}\partial_{\beta_1})f_a^{(1)} + \frac{1}{2}(\partial_{t_1}+\zeta_{a\beta}\partial_{\beta_1})h_a^{(1)}$$
$$= -\frac{1}{\tau\delta_t}f_a^{(2)} + \frac{h_a^{(2)}}{\delta_t}. \tag{4.4c}$$

We have the usual conditions

$$\sum_a f_a = \sum_a f_a^{(eq)} = n, \tag{4.5a}$$

$$\sum_a f_a\zeta_a = \sum_a f_a^{(eq)}\zeta_a = n\vec{u}, \tag{4.5b}$$

$$\sum_a f_a\zeta_{ai}\zeta_{aj} = \sum_a f_a^{(eq)}\zeta_{ai}\zeta_{aj} = n(u_iu_j + \Theta\delta_{ij}), \tag{4.5c}$$

$$\sum_a f_a\zeta_{ai}\zeta_{aj}\zeta_{aj} = n\Theta(u_i\delta_{jk} + u_j\delta_{ki} + u_k\delta_{ij}), \tag{4.5d}$$

where $\Theta = \hat{T}g_{5/2}/g_{3/2}$. For $l \geq 1$, we have

$$\sum_a f_a^{(l)} = 0, \tag{4.6a}$$

$$\sum_a f_a^{(l)}\zeta_a = 0. \tag{4.6b}$$

4.1 Lattice continuity equation and $h_a^{(1)}$

We take the moment of Eqs. (4.4b) and (4.4c), the different order mass conservation equations are recovered below:

$$\partial_{t_1}\sum_a f_a^{(0)} + \partial_{\beta_1}\sum_a f_a^{(0)}\zeta_{a\beta} = -\frac{1}{\tau}\sum_a f_a^{(1)} + \sum_a h_a^{(1)}, \tag{4.7a}$$

$$\partial_{t_2} \sum_a f_a^{(0)} + \sum_a \Big[\frac{1}{2}(\partial_{t_1} + \zeta_{a\beta}\partial_{\beta_1}) h_a^{(1)} - \frac{1}{\delta_t} h_a^{(2)}\Big] = 0. \tag{4.7b}$$

If we set the following constraint

$$\sum_a \Big[\frac{1}{2}(\partial_{t_1} + \zeta_{a\beta}\partial_{\beta_1}) h_a^{(1)} - \frac{1}{\delta_t} h_a^{(2)}\Big] = 0, \tag{4.8}$$

we have

$$\partial_{t_2} \sum_a f_a^{(0)} = 0. \tag{4.9}$$

We have the conservation of mass, i.e., the continuity equation

$$\partial_t n + \delta_t \partial_\beta (n u_\beta) = \sum_a h_a^{(1)}. \tag{4.10}$$

In view of matching the target dynamics Eqs. (2.4a) and (2.5), the selection of $h_a^{(1)}$ becomes obvious

$$h_a^{(1)} = -\frac{w_a n u_r}{r} \delta_t. \tag{4.11}$$

With this choice of $h_a^{(1)}$, the RHS of Eq. (4.10) takes the desired form

$$\sum_a h_a^{(1)} = -\frac{n u_r}{r}. \tag{4.12}$$

4.2 Lattice momentum equation and $h_a^{(2)}$

Next we will determine $h_a^{(2)}$ with $h_a^{(1)}$ specified. After multiplication with ζ_{ai} and summation with respect to a, the different order momentum conservation equations are recovered below:

$$\sum_a \zeta_{ai} h_a^{(2)} = \delta_t \Big(1 - \frac{1}{2\tau}\Big) \partial_{x_j} \sum_a \zeta_{ai}\zeta_{aj} f_a^{(1)} + \delta_t \partial_{t_2} n u_i + \frac{\delta_t}{2} \partial_{x_j} \Big(-\frac{n u_r \delta_t}{r}\Big) \delta_{ij}. \tag{4.13}$$

We first examine the term $\sum_a \zeta_{ai}\zeta_{aj} f_a^{(1)}$ and with Eq. (4.5c). Observe

$$\begin{aligned}\sum_a \zeta_{ai}\zeta_{aj} f_a^{(1)} =& -\tau\delta_t \partial_{t_1} \Big(\sum_a \zeta_{ai}\zeta_{aj} f_a^{(0)}\Big) - \tau\delta_t \partial_{x_k} \Big[n\Theta(u_i\delta_{jk} \\ &+ u_j\delta_{ki} + u_k\delta_{ij}) - \tau\delta_t \frac{n u_r}{r}\Big]\delta_{ij}. \end{aligned} \tag{4.14}$$

Assume the characteristic velocity, length and time of the flow problem are U_c, L_c and t_c, respectively. Then $\partial_{t_1}(\sum_a \zeta_{ai}\zeta_{aj} f_a^{(0)})$ is of order U_c^2/t_c and $\partial_{x_k}\big(n\Theta(u_i\delta_{jk}+u_j\delta_{ki}+u_k\delta_{ij})\big)$ is of order U_c/L_c, and we have

$$\frac{\partial_{t_1}\sum_a \zeta_{ai}\zeta_{aj} f_a^{(0)}}{\partial_{x_k} n\Theta(u_i\delta_{jk}+u_j\delta_{ki}+u_k\delta_{ij})}=\mathcal{O}(M^2). \tag{4.15}$$

Under the assumption $M \ll 1$, one can neglect the term $\partial_{t_1}\sum_a \zeta_{ai}\zeta_{aj} f_a^{(0)}$ to obtain

$$\sum_a \zeta_{ai}\zeta_{aj} f_a^{(1)} = -\tau\delta_t n\Theta(\partial_{x_j}u_i+\partial_{x_i}u_j)+\tau\delta_t\frac{nu_r}{r}(\Theta-1)\delta_{ij}. \tag{4.16}$$

Substituting the above equation into Eq. (4.13), we obtain

$$\begin{aligned}\sum_a \zeta_{ai} h_a^{(2)} =& -\delta_t^2\tau n\Theta\Big(1-\frac{1}{2\tau}\Big)\Big(\frac{\partial^2 u_i}{\partial x_j^2}+\frac{\partial^2 u_j}{\partial x_i\partial x_j}\Big)\\ &+\delta_t^2\Big(1-\frac{1}{2\tau}\Big)\frac{\partial}{\partial x_j}\frac{\tau n u_r}{r}(\Theta-1)\delta_{ij}+\delta_t\frac{\partial}{\partial_{t_2}}nu_i-\frac{\delta_t^2}{2}\frac{\partial}{\partial x_i}\frac{nu_r}{r}.\end{aligned} \tag{4.17}$$

Using the relationship

$$\frac{\partial}{\partial t_1}nu_i=-\frac{\partial}{\partial x_j}n(\Theta\delta_{ij}+u_iu_j), \tag{4.18}$$

and after some algebra, we have

$$\begin{aligned}&n\delta_t\Big(\frac{\partial u_i}{\partial t}+\frac{\partial(u_iu_j)}{\partial x_j}+\frac{1}{n}\frac{\partial P}{\partial x_i}-\mu\frac{\partial^2 u_i}{\partial x_j^2}\Big)\\ =&-n\delta_t\mu\frac{\partial}{\partial x_i}\frac{u_r}{r}-\delta_t^2\Big(\frac{n\mu}{\delta_t}-n\tau\Big)\frac{\partial}{\partial x_i}\frac{u_r}{r}+\sum_a\zeta_{ai}h_a^{(2)},\end{aligned} \tag{4.19}$$

where

$$\mu=\delta_t\Big(\tau-\frac{1}{2}\Big)\Theta.$$

We have $h_a^{(2)}$

$$h_a^{(2)}=n\Big[\delta_t\Big(-\frac{u_ru_j}{r}+\frac{\nu}{r}\frac{\partial u_j}{\partial r}-\frac{\nu u_r}{r^2}\delta_{ir}\Big)\zeta_{aj}w_a+(2\delta_t\mu-\delta_t^2\tau)w_a\zeta_{aj}\frac{\partial}{\partial x_j}\frac{u_r}{r}\Big], \tag{4.20}$$

and we also have

$$h_a^{(2)}=\frac{\delta_t^2}{2}nw_a\Big(\frac{\partial\Theta}{\partial r}+\frac{\partial}{\partial x_j}u_ru_j\Big). \tag{4.21}$$

Finally, we obtain

$$\begin{aligned} h_a^{(2)} =& \frac{\delta_t^2}{2} n w_a \Big(\frac{\partial}{\partial r}\Theta + \frac{\partial}{\partial x_j} u_r u_j \Big) + n\delta_t \Big(-\frac{u_r u_j}{r} + \frac{\mu}{r}\frac{\partial u_j}{\partial r} - \frac{\mu u_r}{r^2}\delta_{ir} \Big) \zeta_{aj} w_a \\ &+ n(2\delta_t \mu - \delta_t^2 \tau) w_a \zeta_{aj} \frac{\partial}{\partial x_j}\frac{u_r}{r}. \end{aligned} \tag{4.22}$$

Regroup the term $h_a^{(2)}$, we finally have

$$\begin{aligned} h_a^{(2)} =& \frac{\partial u_r}{\partial r}\Big[\delta_t n w_a u_r + \frac{n w_a \zeta_{ar}}{r} + \frac{n w_a \zeta_{ar}(2\mu - \delta_t \tau)}{r} \Big]\delta_t + \frac{\partial u_z}{\partial r}\Big[\frac{n w_a \mu \zeta_{az}}{r} \Big]\delta_t \\ &+ \frac{\partial u_r}{\partial z}\Big[\frac{1}{2} n w_a u_z \delta_t + \frac{n w_a \zeta_{az}(2\mu - \delta_t \tau)}{r} \Big]\delta_t + \frac{\partial u_z}{\partial z}\frac{1}{2}\delta_t^2 n w_a u_r \\ &- n w_a \delta_t \Big[\frac{u_r^2 \zeta_{ar}}{r} + \frac{u_r u_z \zeta_{az}}{r} + \frac{\mu u_r \zeta_{ar}}{r^2} + \frac{u_r \zeta_{ar}(2\mu - \delta_t \tau)}{r^2} \Big]. \end{aligned} \tag{4.23}$$

The derivative terms in the above equation can be evaluated using the following

$$\frac{\partial u_r}{\partial r} = \frac{1}{2}\Big[-\frac{1}{\tau n \Theta}\sum_a \zeta_{ar}\zeta_{ar} f_a^{(1)} + \frac{u_r}{r}(1 - \frac{1}{\Theta}) \Big], \tag{4.24a}$$

$$\frac{\partial u_z}{\partial z} = \frac{1}{2}\Big[-\frac{1}{\tau n \Theta}\sum_a \zeta_{az}\zeta_{az} f_a^{(1)} + \frac{u_r}{r}(1 - \frac{1}{\Theta}) \Big], \tag{4.24b}$$

$$\frac{\partial u_z}{\partial r} = \frac{1}{2}\Big[-\frac{1}{\tau n \Theta}\sum_a \zeta_{az}\zeta_{ar} f_a^{(1)} + \frac{u_r}{r}(1 - \frac{1}{\Theta}) \Big], \tag{4.24c}$$

$$\Big(\frac{\partial u_r}{\partial z}\Big)_{r,z} = \frac{(u_r)_{r,z+1} - (u_r)_{r,z-1}}{2\delta_z}. \tag{4.24d}$$

It is noted that only one derivative term has to be computed using finite (central) difference method and the rest of derivative terms can be analytically expressed and directly computed. To complete the derivation, we set

$$h_a = \delta_t h_a^{(1)} + \delta_t^2 h_a^{(2)},$$

in Eq. (4.1) to achieve the final semiclassical axisymmetric lattice Boltzmann method.

In summary, Eqs. (4.1), (4.11) and (4.23) form a closed set of differential equations governing the set of variables $f_a(\vec{x}, t)$ in the physical configuration space. Once we have solved the new time values of $f_a(\vec{x}, t)$, the macroscopic variables such as $n(\vec{x}, t), \vec{u}(\vec{x}, t)$ and $\hat{T}(\vec{x}, t)$, can be calculated by

$$n(\vec{x}, t) = \sum_{a=1}^{l} f_a(\vec{x}, t), \tag{4.25a}$$

$$n\vec{u} = \sum_{a=1}^{l} f_a \vec{\zeta}_a, \tag{4.25b}$$

$$n\Big(D\hat{T}\frac{g_{\frac{5}{2}}(z)}{g_{\frac{3}{2}}(z)} + u^2 \Big) = \sum_{a=1}^{l} f_a \zeta_a^2 = E. \tag{4.25c}$$

The above three equations provide a way to determine the fugacity z through an iteration method

$$E - 3\left(\frac{n}{g_{\frac{3}{2}}}\right)^{\frac{5}{3}} g_{\frac{5}{2}} - nu^2 = 0. \tag{4.26}$$

After obtaining z, we can get the temperature $\hat{T}$.

To apply Eq. (4.1), one has to determine either τ or τ^*. For continuum flows, one can perform Chapman-Enskog multiscale analysis to Eq. (4.1) and τ is determined in such a way that the Navier-Stokes equations are recovered. As a result, we have the relaxation time τ related to the fluid viscosity ν as

$$\nu = \left(\tau - \frac{1}{2}\right)\hat{T}\frac{g_{\frac{5}{2}}}{g_{\frac{3}{2}}}, \tag{4.27}$$

where ν is the non-dimensional kinematic viscosity. The term $-1/2$ in the above equation is a correction to make the LBE technique a second-order method for solving incompressible flows.

5 Results and discussion

To illustrate the present method, we consider a standard uniform disturbance-free flow with velocity $\vec{U}_\infty$ over a sphere in a quantum gas. The diameter of the sphere is D and Reynolds number is defined as

$$Re_\infty = \left|\vec{U}_\infty\right|\frac{D}{\nu}.$$

We consider two cases with Re_∞=20 and Re_∞=40, respectively. The state of flow is fully laminar with steady separation and enclosed near wake structure and the flow pattern is symmetric. The kinematic viscosity ν can be obtained from the given Reynolds number and the relaxation time τ, which is calculated according to Eq. (4.27). The computational domain is $(-1,1) \times (-1,1)$ and is divided into 201×201 uniform lattices and the sphere is set at the center of the domain and with diameter D=0.1. The equilibrium distribution function with the given uniform free stream conditions is used to implement the boundary conditions at the far fields and at the sphere surface. A boundary treatment using immersed boundary velocity correction method proposed in [29–33], which enforce the physical boundary condition, is also adopted here. We used the N=3 expansion equations set for all the cases computed.

The steady streamline patterns for the three statistics, BE, MB and FD gases for the case of z=0.2 and Re_∞=20 are shown in Fig. 1, respectively. For this low Reynolds number, the flow pattern is steady, laminar, symmetric and closed near-wake is formed. The weak recirculating flow in the near-wake contains vigorous twin vortices and the size of the twin vortices or eddies is larger for the FD gas and smaller for the BE gas as compared with that of the MB gas.

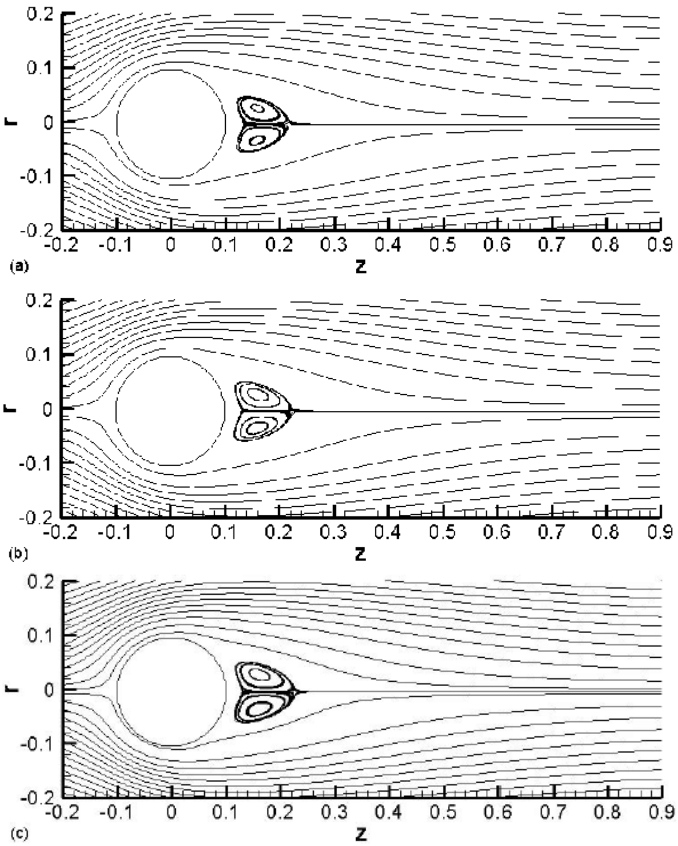

Figure 1: Streamlines of uniform flow over a sphere in a quantum gas with $z = 0.2$ and $Re_\infty = 20$. (a) BE gas, (b) MB gas, (c) FD gas.

Similarly, the corresponding results for the case Re_∞=40 are shown in Fig. 2. The flow patterns are symmetric and the enclosed near-wake becomes elongated and larger and may become unstable when Re_∞ is getting higher. The size of wake vortices becomes much larger as compared with that of Re_∞=20 case. Again, the recirculation region is larger for the FD gas, smaller for the BE gas while that for the MB gas always lies in between. This reflects the fact that the Maxwell-Boltzmann distribution always lies in between the Bose-Einstein and Fermi-Dirac distributions as delineated by the θ value in Eq. (2.2). According to quantum statistics, the effects of quantum statistics at finite temperatures (non-degenerate case) are approximately equivalent to introducing an interaction between particles [34]. This interaction is attractive in nature for bosons and repulsive for femions and operates over distances of order of the thermal de Broglie wavelength Λ. The present results seem to be able to illustrate and explore the manifestation of the effect of quantum statistics macroscopically. Finally, it is noted that as compared with the flow over 2-D circular cylinder presented in [16], the size of the near-wake recirculation zone of 2-D cylinder case is always larger than the corresponding axisymmetric sphere case due to the three-dimensional relieving

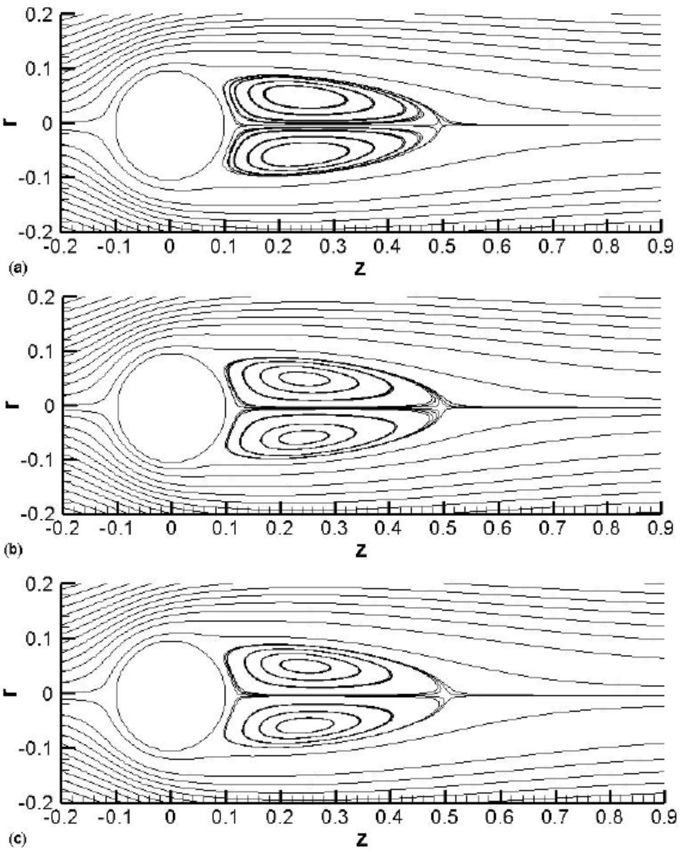

Figure 2: Streamlines of uniform flow over a sphere in a quantum gas with $z = 0.2$ and $Re_\infty = 40$. (a) BE gas, (b) MB gas, (c) FD gas.

effect for the axisymmetric sphere case. In quantitative comparisons of these three statistics, we found the drag coefficients of the sphere in the Bose-Einstein, Maxwell-Boltzmann and Fermi-Dirac statistics are 1.804, 1.739 and 1.685, respectively. Also, the corresponding wake lengths are found to be equal to 0.492, 0.497 and 0.5, respectively.

6 Conclusions

The flows of gases of particles of arbitrary statistics in an axisymmetric flow are investigated using a newly developed semiclassical lattice Uehling-Uhlenbeck Boltzmann-BGK method. The method is derived based on a previous two-dimensional nine-velocity D2Q9 semiclassical lattice Boltzmann method and the forcing strategy of Halliday et al. [17] by adding forcing terms to modify the the emergent macroscopic equations toward axisymmetric governing equations. The detailed derivation of the forcing terms is presented. The equilibrium distribution of lattice Boltzmann equations 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. Moreover, our development recovers previous classical results when the classical limit is taken. Computations of uniform flow over a sphere in both Bose-Einstein and Fermi-Dirac gases have been simulated to illustrate the method. From the streamline patterns and recirculation zones, 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. Our results are obtained based on a systematic and parallel treatment of all statistics, hence it can be self checked with the theory consistently among the three statistics.

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