INPE – National Institute for Space Research
São José dos Campos – SP – Brazil – May 16-20, 2016

THERMAL LATTICE BOLTZMANN METHOD FOR DILUTE FLUIDS OF BOSONS AND FERMIONS

Rodrigo C. V. Coelho[1], *Anderson S. Ilha*[2], *Mauro M. Doria*[3]

[1]Universidade Federal do Rio de Janeiro (UFRJ), Rio de Janeiro, Brazil. rcvcoelho@if.ufrj.br
[2]Instituto Nacional de Metrologia, Qualidade e Tecnologia (INMETRO), Rio de Janeiro, Brazil. anderson.ilha@gmail.com
[3]Universidade Federal do Rio de Janeiro (UFRJ), Rio de Janeiro, Brazil. mmd@if.ufrj.br

Abstract: A thermal lattice Boltzmann method is developed to semi-classically treat a dilute gas of bosons and fermions. For our model, we expand the Bose-Einstein and Fermi-Dirac distributions up to fourth order in Hermite polynomials and we use the approximation of small fugacity to expand the integrals. The simulations are performed in a two dimensional system which has a circle in the center with higher density and the conservation of energy is analyzed.

keywords: Fluid dynamics, Plasma and Turbulence; Modeling, Numerical Simulation and Optimization; Nonlinear Dynamics in Thermal and Fluid Sciences

1. INTRODUCTION

The lattice Boltzmann method (LBM) is a computational fluid dynamics technique which has been extensively used in industry and research for the last two decades to simulate, mostly, classical fluids[8]. It is based on the Boltzmann equation with the Bhatnagar-Gross-Krook collision operator[5],

$$f_\alpha(\boldsymbol{x}+\boldsymbol{e}_\alpha, t+1) - f_\alpha(\boldsymbol{x}, t) = -\frac{f_\alpha(\boldsymbol{x}, t) - {f^{(eq)}}_\alpha(\boldsymbol{x}, t)}{\tau},$$

and on the Gaussian quadrature. The model was also extended to relativistic fluids in 2010[7] and, thenceforth, it was successfully applied to many relativistic systems[3, 6]. Nevertheless, few models have been proposed for semi-classical fluids, governed by the Bose-Einstein (BE) and Fermi-Dirac (FD) statistics. In 2009, Yang and Hung proposed thermal model for semi-classical fluids[11] by expanding the BE and

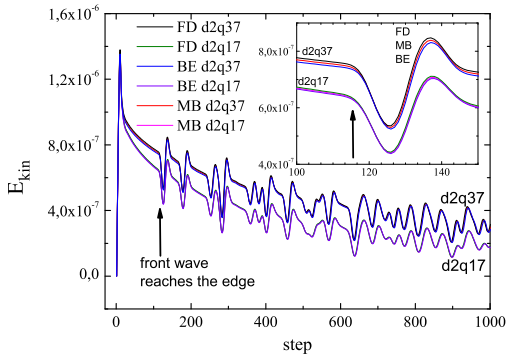

Figure 1 – The Kinetic energy of the FD, MB and BE distributions using the D2V17 and D2V37 lattices is shown here for the first 1000 time steps. The initial condition used is of the circle of density. The inset shows in a particular time step window the splitting of the kinetic energy among the three distributions for both D2V17 and D2V37 lattices.

FD distributions up to third order in Hermite polynomials. In 2014, Coelho et. al. [2] demonstrated that the correct thermodynamics in a thermal LBM, even for classical case, can only be recovered by expanding the distribution function up to fourth order. The authors also obtained the correct conservation laws of mass, momentum and energy for semi-classical fluids of bosons and fermions. In 2015, Coelho, Ilha and Doria [1] developed a more general LBM for semi-

classical fluids based on the discovery of a new polynomial base more generic than the Hermite one, but this work will not be considered in this extended abstract.

2. PURPOSE

Here we describe the LBM used to simulated dilute gases of bosons and fermions. For more details see Coelho et. al. 2014 [2]. First, the BE-FD distribution function,

$$f^{(0)}(\boldsymbol{\xi}) = \frac{1}{z^{-1}\exp\left[\frac{(\boldsymbol{\xi}-\boldsymbol{u})^2}{2\theta}\right]\pm 1}, \tag{1}$$

is expanded up to fourth order in Hermite polynomials. The fourth order expansion is necessary to build a correct thermal model. After some algebra, we obtain:

$$\begin{aligned} f_\alpha^{(eq)} &= w_\alpha\rho\Bigg\{1+(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})\left(1-\frac{1}{2}\boldsymbol{u}^2\right)+\frac{1}{6}(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})^3 \\ &+(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})^2\left(\frac{1}{2}-\frac{1}{4}\boldsymbol{u}^2\right)-\frac{1}{2}\boldsymbol{u}^2+\frac{1}{8}\boldsymbol{u}^4 \\ &+\frac{1}{24}(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})^4+\left(\bar{\theta}-1\right)\cdot\Bigg[\frac{1}{2}(\boldsymbol{\xi}_\alpha^2-D) \\ &+\frac{1}{2}(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})(\boldsymbol{\xi}_\alpha^2-D-2)+\frac{1}{4}(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u})^2(\boldsymbol{\xi}_\alpha^2 \\ &-D-4)+\frac{1}{4}\boldsymbol{u}^2(D+2-\boldsymbol{\xi}_\alpha^2)\Bigg]+\frac{1}{8}\left[\bar{\theta}^2 g(z)\right. \\ &\left.-2\bar{\theta}+1\right]\cdot[\boldsymbol{\xi}_\alpha^4+(D+2)(D-2\boldsymbol{\xi}_\alpha^2)]\Bigg\}, \end{aligned} \tag{2}$$

where the function $g(z)$ is defined in Eq.10 and moments are defined by

$$\rho(\boldsymbol{x}) \equiv \int d^D\boldsymbol{\xi}\; f^{(0)}(\boldsymbol{\xi}), \tag{3}$$

$$\boldsymbol{u}(\boldsymbol{x}) = \frac{1}{\rho(\boldsymbol{x})}\int d^D\boldsymbol{\xi}\;\boldsymbol{\xi} f^{(0)}(\boldsymbol{\xi}), \text{ and} \tag{4}$$

$$\frac{D}{2}\bar{\theta}(\boldsymbol{x}) = \frac{1}{\rho(\boldsymbol{x})}\int d^D\boldsymbol{\xi}\;\frac{1}{2}\left[\boldsymbol{\xi}-\boldsymbol{u}(\boldsymbol{x})\right]^2 f^{(0)}(\boldsymbol{\xi}). \tag{5}$$

We develop the approximation of the dilute semi-classical (BE-FD) system, which is very close to the classical (MB) limit. This is the limit of small fugacity, $z = e^{\mu/\theta} \ll 1$ taken in the BE-FD integrals [9]:

$$\begin{aligned} g_\nu(z) &\equiv \frac{1}{\Gamma(\nu)}\int_0^\infty \frac{x^{\nu-1}\,dx}{z^{-1}e^x\pm 1} &(6)\\ &= g_\nu(z) = z\mp\frac{z^2}{2^\nu}+\cdots &(7)\end{aligned}$$

where the assignment is (+) BE and (-) FD, respectively. We are going to carry here just the first order corrections to the classical (MB) fluid which are linear in the fugacity. In this order the density and the pseudo temperature are given by,

$$\rho \equiv (2\pi\theta)^{\frac{D}{2}} g_{\frac{D}{2}}(z) = (2\pi\theta)^{\frac{D}{2}}\, z+\cdots \tag{8}$$

$$\bar{\theta} \equiv \theta\frac{g_{\frac{D}{2}+1}(z)}{g_{\frac{D}{2}}(z)} = \theta\left(1\pm\frac{z}{2^{\frac{D}{2}+2}}+\cdots\right). \tag{9}$$

Note that the density is not an independent parameter as in classical case. Within this order we can write the fugacity and so the function $g(z)$, that appear in terms of the density and of the pseudo temperature,

$$g(z) \equiv \frac{g_{\frac{D}{2}}(z)\cdot g_{\frac{D}{2}+2}(z)}{\left(g_{\frac{D}{2}+1}(z)\right)^2} \approx 1\mp\frac{1}{2^{\frac{D}{2}+2}}\frac{\rho}{\left(2\pi\bar{\theta}\right)^{\frac{D}{2}}} \tag{10}$$

under the assumption that $z \approx \rho/\left(2\pi\bar{\theta}\right)^{\frac{D}{2}} \ll 1$. Under this approximation the function g can be brought back to the BE-FD equilibrium distribution function, Eq.2, that becomes a function of ρ, $\bar{\theta}$ and $\boldsymbol{u}$.

Thus the LBM for the dilute quantum fluid can be developed through the variables density ρ, macroscopic velocity $\boldsymbol{u}$ and pseudo temperature $\bar{\theta}$. The latter is related to the true temperature θ through the relation,

$$\bar{\theta} \approx \theta \pm \frac{\rho}{16\pi}, \tag{11}$$

where the $+$ and $-$ signs applies to fermions and bosons, respectively.

3. RESULTS AND DISCUSSION

In this section we use the LBM based on the present $N = 4$ order theory to numerically solve the dilute semi-classical fluid. We find that the energy is indeed conserved in $D = 2$ under periodic boundary conditions and some initial conditions that trigger a time evolution where motion and heat occur simultaneously. The initial conditions are associated to a circle of radius R located at the center of the cell where the density ρ assumes a special value, whereas the velocity and temperature are taken constant throughout the cell. We work with a grid of $A_{cell} = 256^2$ points, and in these units $R = 10$. We take for the relaxation time $\tau t = 0.58$. We use in this section the concept of a real temperature T connected to the reduced one by $T \equiv c_s^2\theta$, where c_s is a distinct numerical parameter for each of the lattices D2V17 and D2V37[2]. Since our goal is to verify that the total energy remains constant in the cell at any time step, we define the following sums over all cell points, which are the average values of the kinetic and the thermal energies in the cell:

$$E_{kin} \equiv \frac{1}{A_{cell}}\sum_{cell}\frac{1}{2}\rho\boldsymbol{u}^2 \tag{12}$$

$$E_{therm} \equiv \frac{1}{A_{cell}}\sum_{cell}\frac{D}{2}\rho\bar{\theta}, \text{ and} \tag{13}$$

$$E_{total} \equiv E_{kin}+E_{therm}. \tag{14}$$

In our numerical study we assume identical initial conditions for the BE, FD and MB cases, which means that they start with the same density, temperature and velocity. Thus the initial kinetic energy of Eq.(12) is the same for the three cases, but not the thermal energy of Eq.(13) since the initial pseudo temperature is not the same for the three cases, according to Eq.(11), being greater for fermions and smaller for bosons, as compared to the classical case.

Under the initial condition the density is $\rho = 0.12$ inside and $\rho = 0.1$ outside the circle of radius $R = 10$. The initial temperature is $T = 0.5$ and the macroscopic velocity $\boldsymbol{u}$ is zero everywhere. Though there is no initial motion, the non homogeneous density distribution sets a pressure front. The higher density at the center means higher pressure that forces motion outward the circle, and so, generates friction, heating and raise of the temperature in the cell. The first 1000 steps of E_{kin} are shown in Fig. 1. Notice that it starts from zero and the oscillatory behavior set by the entrance of wave fronts from neighbor cells is well described by the D2V17 and D2V37 lattices since their numerical differences are in the range of 10^{-7}. In this case too the difference among the three distributions is hidden by the lattice difference, shown in the inset for a chosen window of time steps for both lattices. The trend towards kinetic energy decay is seen in this figure though the convergence towards a steady state is only suggested by this figure. To really see it a larger window must be taken. The time step evolution of E_{therm} is shown in Fig.(2). E_{therm} experiments a sudden drop to allow for the increase of E_{kin} (Fig.(1)) as the system starts motion due to pressure unbalance. As in the previously case, E_{total} is

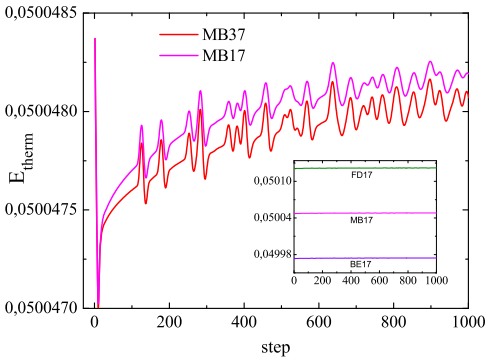

Figure 2 – The thermal energy of the MB distribution using the D2V17 and D2V37 lattices is shown here for the first 1000 time steps. The initial condition used is that of the circle of density. The inset shows in a particular time step window the splitting of the kinetic energy among the three distributions for the D2V17 lattice.

absolutely conserved to machine precision, in our case tested to order 10^{-10}. The inset of this plot shows the splitting of the three distributions within the first 1000 steps. Notice that such values are distinct because we chose the same initial θ for the three distributions, which means different $\bar{\theta}$ in the three cases. Finally we address the evolution of the temperature deviation from its initial value $T = 0.5$ in Fig.(3) within the full time step window studied, namely 20000 steps. The very first 20 steps, shown in the inset, indicate that the initial temperature is the same in all cases. However the final ones are different. The D2V17 reaches a final temperature deviation at a value slightly lower that the D2V37 case by an order of magnitude of 10^{-7}. The final deviation is higher for the FD distribution and lower for the BE. We notice during evolution a drop to a minimum of temperature required to accommodate the kinetic expansion caused by the pressure unbalance in an energy conserving scenario.

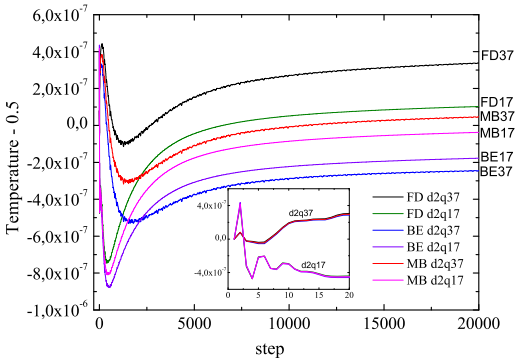

Figure 3 – The temperature deviation from its initial value is shown here for the case of a circle of density as initial condition for the first 20000 time steps. The curves for the three distributions and the two lattices are clearly seen here. The inset shows the first 20 time steps.

4. CONCLUSION

In this work, we described our thermal LBM for semi-classical dilute fluids of bosons and fermions and we performed a simple simulation to verify the conservation of the total energy. Our code converges and produces realistic results for regimes near to the classical one, i.e., regimes weakly semi-classical. The merit of this model is to correctly describe the thermodynamics of the system, what can only be done by expanding the distribution function up to fourth order, as demonstrated in Ref.[2]. The success of this model represent an important contribution to the understanding of the thermal LBM and the semi-classical LBM, both with lack of contributions.

ACKNOWLEDGMENTS

Rodrigo C. V. Coelho thanks to CNPq and FAPERJ for financial support and M.M.D. acknowledges CNPq support from funding 23079.014992/2015-39.

REFERENCES

References

[1] R. C. V. Coelho, A. Ilha, and M. M. Doria. A lattice Boltzmann method based on generalized polynomials. *ArXiv e-prints*, October 2015.

[2] Rodrigo C. V. Coelho, Anderson Ilha, Mauro M. Doria, R. M. Pereira, and Valter Yoshihiko Aibe. Lattice boltzmann method for bosons and fermions and the fourth-order hermite polynomial expansion. *Phys. Rev. E*, 89:043302, Apr 2014.

[3] O. Furtmaier, M. Mendoza, I. Karlin, S. Succi, and H. J. Herrmann. Rayleigh-bénard instability in graphene. *Phys. Rev. B*, 91:085401, Feb 2015.

[4] H. Ibach and H. Lüth. *Solid-State Physics: An Introduction to Principles of Materials Science ; with 100 Problems*. Advanced texts in physics. Springer, 2003.

[5] G.M. Kremer. *An Introduction to the Boltzmann Equation and Transport Processes in Gases*. Interaction of Mechanics and Mathematics. Springer Berlin Heidelberg, 2010.

[6] M. Mendoza, B. M. Boghosian, H. J. Herrmann, and S. Succi. Derivation of the lattice boltzmann model for relativistic hydrodynamics. *Phys. Rev. D*, 82:105008, Nov 2010.

[7] M. Mendoza, B. M. Boghosian, H. J. Herrmann, and S. Succi. Fast lattice boltzmann solver for relativistic hydrodynamics. *Phys. Rev. Lett.*, 105:014502, Jun 2010.

[8] A. A. Mohamad. *Lattice Boltzmann Method*. Springer, London, 2011.

[9] R.K. Pathria. *Statistical Mechanics*. 1996.

[10] Eleuterio Toro. *Riemann Solvers and Numerical Methods for Fluid Dynamics - A Practical Introduction*. 2009.

[11] Jaw-Yen Yang and Li-Hsin Hung. Lattice uehling-uhlenbeck boltzmann-bhatnagar-gross-krook hydrodynamics of quantum gases. *Phys. Rev. E*, 79:056708, May 2009.