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A LATTICE BOLTZMANN METHOD FOR ELECTRONS IN METALS

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Abstract: Recently, we discovered a new tensorial polynomial base which allow a new approach to model semi-classical fluids using lattice Boltzmann. In this work, we apply this method for electrons in metals at zero temperature. We tested our model numerically using the shock tube test and the Poiseuille flow. This kind of model can be the first step to simulate microelectronic transport.

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[11]. It is based on the Boltzmann equation with the Bhatnagar-Gross-Krook collision operator[8],

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

and on the Gaussian quadrature. The model was also extended to relativistic fluids in 2010[10] and, thenceforth, it was successfully applied to many relativistic systems[5, 9]. 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[13] by expanding the BE and FD distributions up to third order in Hermite polynomials. In 2014, Coelho et. al. pointed out that a correct thermal model, even for classical fluids, can only be obtained by expanding the distribution function up to fourth order, obtained the macroscopic equations for mass, momentum and energy conservation and applied the model for a dilute gas of bosons and fermions[4]. The problem with these two models is that they use the Hermite polynomials, what restricts it for regimes near to classical (like a dilute gas). In 2015, Coelho, Ilha and Doria proposed the first general model (not published yet) capable to model semi-classical fluids in any regime [3] due to the discovery of a new polynomial base of orthogonal polynomials in D dimensions.

The application we develop in this work using this LBM based on generalized polynomials is for electrons in metals. It is well-known that the Boltzmann-BGK equation provides the framework to understand the Drude-Sommerfeld model which is the standard textbook procedure to treat the transport of electrons in metals. [1, 7]. Electrons form a gas, similarly to the atoms in a rarefied gas, however at room temperature they are essentially governed by their zero temperature properties, and so the Fermi speed v_F is important (for instance, for cooper [1], $v_F = 1.57\ 10^6$ m/s). The displacement velocity is very low in metals, for common electric fields, $u \sim$ 0.1-1.0 m/s, that is, $u/v_F \sim$ 6.4-64 10^{-8}, while Mach's number diverges for $T = 0$. The new polynomials bring a new velocity scale, c_0, that can even be *local* whereas c_r is necessarily global, and so, provide clear advantage over previous methods. The novel LBM will bring advances in areas such as microelectronics since it allows for the treatment of the electron gas in any geometrical ar-

rangement under the presence of impurities, inhomogeneous fields and temperature gradients. Since the electronic mean free path l falls in the sub-micrometer range (the collision time of cooper [1] is $\tau = 2.1\,10^{-13}$ s and $l = v_F\tau \sim 0.33$ μm) the macroscopic equations of motion of continuum fluid mechanics obtained from this novel LBM become useful [4] (small Knudsen number, $Kn \sim l/L$, L is the typical length scale of the system).

2. PURPOSE

In this section, we describe briefly the model used to simulate electrons in metals. For more details, see our arXiv (non-published) Coelho et. al. 2015 [3]. It is based on the discovery of a new base of orthogonal polynomials in D dimensions which allow us to expand a distribution function using a generic weight function. The can not use, for instance, the well known Hermite polynomials because its weight function is a Gaussian, i.e., $\omega(\xi) = \exp(-x^2/2)/(2\pi)^{\frac{D}{2}}$, which is not appropriate to expand the FD function, that is closer to step function for low temperatures. Thus we expand the FD distribution,

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

up to third order in this polynomial base using the distribution function itself with $\boldsymbol{u} = 0$ as the weight function. Note that in this procedure we keep the temperature θ and the chemical potential μ in the weight, which will not be constant in time and position anymore as happens in all other LBM's (classical and relativistic). It was only possible by the discovery of this new polynomial basis and this approach has good advantages including better numerical convergence and more realistic results. It leads us to

$$\begin{aligned} f_\alpha^{(eq)} = w_\alpha \Bigg\{ & 1 + \frac{I_0}{I_2}\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u} + \frac{I_0}{2I_4}\left(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u}\right)^2 - \\ & \frac{I_0\left(\Delta_2^2-1\right)}{2I_4 D}\boldsymbol{u}^2\boldsymbol{\xi}_\alpha^2 - \frac{I_2}{2I_4}\Delta_2^2\boldsymbol{u}^2 + \frac{1}{6}I_0\left(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u}\right)\cdot \\ & \Bigg[3\left(1-J_2\right)\frac{J_4}{I_2}\left(D+2\right)\Delta_4^2 - 3\left(1-J_2\right)\frac{J_4}{I_4}\Delta_4^2\boldsymbol{\xi}_\alpha^2 - \\ & -3\frac{J_4}{I_4}\Delta_4^2\boldsymbol{u}^2 + 3\frac{\Delta_4^2-1}{I_6\left(D+2\right)}\boldsymbol{\xi}_\alpha^2\boldsymbol{u}^2 + \frac{1}{I_6}\left(\boldsymbol{\xi}_\alpha\cdot\boldsymbol{u}\right)^2\Bigg]\Bigg\}, \end{aligned}$$

where the I_N's are integrals of the weight function defined by

$$\int d^D\boldsymbol{\xi}\,\omega(\boldsymbol{\xi})\,\xi_{i_1}\cdots\xi_{i_N} = I_N\,\delta_{i_1\cdots i_N}, \tag{3}$$

$\Delta_L^2 \equiv 2/\left[\left(D+L\right) - J_L\left(D+L-2\right)\right]$ and $J_L \equiv I_L^2/I_{L+2}I_{L-2}$. By symmetry it holds that $I_N = 0$ for N odd. We introduce the following tensors which are sums of products of the Kronecker's delta function ($\delta^{ij} = 1$ for $i = j$ and 0 for $i \neq j$), namely, $\delta_{i_1\cdots i_N|j_1\cdots j_N} \equiv \delta_{i_1 j_1}\cdots\delta_{i_N j_N} +$ all permutations of j's and $\delta_{i_1\cdots i_N\,j_1\cdots j_N} \equiv \delta_{i_1 j_1}\cdots\delta_{i_N j_N} +$ all permutations. Thus they contain $N!$ and $(2N)!$ terms, respectively.

Since the room temperature ($\sim$ 300 K) is much smaller than the Fermi temperature for electrons in metals ($\sim$ 12000 K), the use of Sommerfeld expansion[7] is justified for I_N's,

$$\begin{aligned} I_{2N} = & \frac{(2\pi)^{\frac{D}{2}}\mu^{N+\frac{D}{2}}}{\Gamma\left(N+\frac{D}{2}+1\right)}\cdot \\ & \left[1 + \frac{\pi^2}{6}\left(N+\frac{D}{2}\right)\left(N+\frac{D}{2}-1\right)\left(\frac{\theta}{\mu}\right)^2 + \cdots\right] \end{aligned} \tag{4}$$

and we can expand the weighs for the lattice that will be used in our simulations: d1v3 and d2v9. The *d1v3* ($D = 1$) lattice contains only three velocities, $\boldsymbol{e}_0 = 0$, $\boldsymbol{e}_{\pm1} = \pm1$ and the associated weights are $w_0 = I_0\left(1 - J_2/3\right)$ and $w_{\pm1} = I_0 J_2/6$. The lattice *d2v9* ($D = 2$) has its geometrical velocities on the sides and diagonals of a square, namely, $\boldsymbol{e}_\alpha$, $\alpha = 0,\cdots,8$: $\boldsymbol{e}_0 = (0,0)$, $\boldsymbol{e}_{long} = [(1,1),(1,-1),(-1-1),(1,-1)]$ and $\boldsymbol{e}_{short} = [(1,0),(0,1),(-1,0),(0,-1)]$. The corresponding weights are $w_0 = I_0\left(1 - 5J_2/9\right)$, $w_l = I_0 J_2/36$ and $w_s = I_0 J_2/9$, associated to the center, long and short vectors, respectively. For both lattices $c_0 = \sqrt{3I_4/I_2}$ For simplicity, we choose the temperature as being zero. This renders $I_0 = (2\pi\mu)^{D/2}/\Gamma(D/2+1)$ and $J_2 = (D+4)/(D+2)$. Local changes in ρ and u are only possible due to local variations in the chemical potential. The velocity scale, $c_0 = \sqrt{6\mu/(D+4)}$, is essentially the Fermi velocity. Updates are done in the density and in the normalized velocity,

$$I_0 = \sum_\alpha f_\alpha \boldsymbol{e}_\alpha \;\text{ and }\; \boldsymbol{u}_0 \equiv \frac{\boldsymbol{u}}{c_0} = \frac{1}{I_0}\sum_\alpha f_\alpha \boldsymbol{e}_\alpha. \tag{5}$$

3. RESULTS AND DISCUSSION

Here we show the numerical simulations to test the validity of our LBM for electrons in metals.

The shock tube test - The one-dimensional Navier-Stokes equation is independent of τ because the viscosity stress tensor vanishes for $D = 1$, and so reduces to the Euler equation [4]. A direct comparison between a known solution of the Euler equation in case of a stepwise initial condition, the so-called Riemann problem [12], and our numerical solution of the one-dimensional Boltzmann equation is possible. For both lattices, d1v3 and d2v9, we find independence of the numerical solution with respect to τ within a wide range (τ = 0.57-0.95, reduced units). Fig. 1 shows the comparison between the obtained ρ and u with the known Riemann problem. Fermions at zero temperature obey an isothermal perfect gas law where the temperature is the Fermi temperature itself. Fig. 1 shows this comparison between the shock wave solution for an isothermal gas and the LBM simulations for the lattices *d1v3* and *d2v9* after 500 steps. We find good agreement for the density and velocity curves of the *d1v3* and *d2v9*.

The Poiseuille flow - We also performed the simulation for the Poiseuille flow for electrons. The relation between the velocity in x direction and the height (y) is shown in

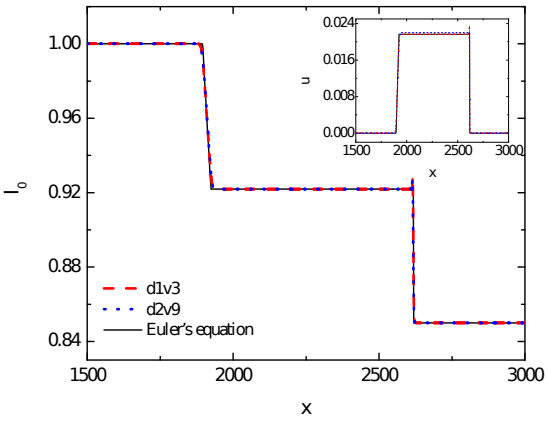

Figure 1 – Simulations are done in a one-dimensional system with $L_X \times L_Y = 3001 \times 1$ nodes with periodic boundary conditions. The initial velocity is zero everywhere and the density is 1.0 for $L_X/4 < x < 3L_X/4$ and 0.85 elsewhere. Only half of the system is shown since the other one is a mirror image. The relaxation time is $\tau = 0.58$.

Fig. 2. As predicted by Navier-Stokes[4] equation, the velocity profile can be fit as a parabola $f(x) = ax^2 + b$ with a good agreement. The obtained coefficients were $a = (-2.222 \pm 0.001) \times 10 - 05$ and $b = (0.12572 \pm 0.00003)$, both in lattice units[11]. In our simulations, the system has the dimensions 501×151, the relaxation time is $\tau = 0.9$ and the code stopped after 10^5 time steps.

It is remarkable that LBM with so many transformations compared to the classical one still converges and produces good results. It shows that our model works as expected and it can be applied to more realistic simulations.

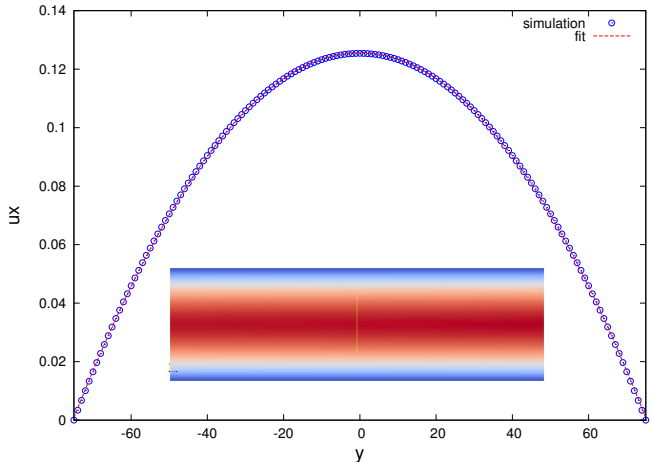

Figure 2 – Velocity profile in Poiseuille flow for electrons in metals. The density in the left boundary is fixed as 1.51, in the right boundary it is 1.49 and in the top and bottom walls the velocity is zero. The inset shows the velocity field with the red color for higher values and the blue for lower values of velocity.

4. CONCLUSION

In summary, we developed a LBM model based on generalized polynomials for a semi-classical gas of electrons in metals. We tested this model using the shock tube test with very good agreement with the analytical solution of Euler equations and we also simulated the Poiseuille flow obtaining a parabolic velocity profile as predicted by Navier-Stokes equation. The simulations performed here were only numerical tests for the computational model and may not correspond to realistic situations. For instance, if we want to simulate a flow of electrons in a wire, the boundary conditions used in Poiseuille flow may not be appropriate and we should not use the non-slip ($\boldsymbol{u} = 0$) condition in top and bottom boundaries. Future tests will involve the recovery of well known physical results as the Ohms'law. This was the first LBM created to model electrons in metals and it represent a significant contribution to computational fluid dynamics. In the future, improved LBM's for electrons can be used in industries and research so commonly as the classical LBM is used presently.

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