A lattice Boltzmann method based on generalized polynomials and its application for electrons in metals

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Abstract – A lattice Boltzmann method is proposed based on the expansion of the equilibrium distribution function in powers of a new set of generalized orthonormal polynomials which are here presented. The new polynomials are orthonormal under the weight defined by the equilibrium distribution function itself. The $D$-dimensional Hermite polynomials is a sub-case of the present ones, associated to the particular weight of a Gaussian function. The proposed lattice Boltzmann method allows for the treatment of semi-classical fluids, such as electrons in metals under the Drude-Sommerfeld model, which is a particular case that we develop and validate by the Riemann problem.

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Introduction. – The lattice Boltzmann method (LBM) has been applied in many problems of classical fluid dynamics ranging from biology to material science [1,2]. Its strength lies in the ability to easily incorporate complex physical phenomena, naturally present in micron scale, porous media, and multiphase flows. The method is implemented on a regular discrete position space, such that the continuum fluid mechanics is retrieved at distances much larger than the lattice scale. Initially conceived as a gas of colliding particles with confined motion along a lattice [3], the LBM quickly reached widespread use once its underlying mathematical structure was understood.

The LBM came to existence long before its connections to the $D$-dimensional Hermite polynomials (DHP) and to the Maxwell-Boltzmann (MB) equilibrium distribution function (EDF) were established [4–6]. Later such connections were understood and brought understanding to the fundamentals of the LBM [7,8]. It was Grad [9,10] who first used the DHP to describe the microscopic velocity space [10] of the Boltzmann equation, but these polynomials are important in other areas as well, such as quantum optics [11]. The LBM has been mostly applied to the MB isothermal fluid [12,13], but recent applications to explain relativistic flows [14] and graphene [15] have revealed a new trend in the LBM, which is to go beyond the standard framework of the DHP and the MB distribution.

In this letter we propose a novel LBM for the treatment of semiclassical fluids that incorporates the previous LBM as a sub-case, and because of its convergent properties it can go beyond in case of the above fluids, specially in situations under complexity. The present advancements are due to our discovery of a new class of $D$-dimensional polynomials. Hence the present proposal opens the way to treat electrons in metals, for instance, through the LBM method, a long expected goal not yet achieved for lackness of the appropriate theoretical tools which are here presented. 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 electrons in metals [16]. 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 velocity \( v_F \), and not the sound velocity, \( c_s \), is important (for instance, for copper [16], \( v_F = 1.57 \times 10^6 \text{ m/s} \)). The displacement velocity is very low in metals, for typical electric fields, \( u \approx 0.1-1.0 \text{ m/s} \), that is, \( u/v_F \approx 6.4-64 \times 10^{-8} \), 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. Therefore, they provide clear advantage over previous methods. The novel LBM will bring advances in areas such as microscale electronics since it allows for the treatment of the electron gas in any geometrical arrangement under the presence of inhomogeneous fields, temperature gradients and defects. Since the electronic mean free path \( l \) falls in the sub-micrometer range (the collision time of copper [16] is \( \tau = 2.1 \times 10^{-13} \text{ s} \) and \( l = v_{TF} \tau \approx 0.33 \mu \text{ m} \)), the macroscopic equations of motion of continuum fluid mechanics obtained from this novel LBM become useful [17] (small Knudsen number, \( Kn \approx l/L \), \( L \) is the characteristic length scale of the system).

Semi-classical fluids have particles that obey either the Fermi-Dirac (FD) or the Bose-Einstein (BE) statistics, and only for low densities and high temperatures they become the well-known MB statistics satisfied by the atoms in a gas. Long ago Uhlen and Uhlenbeck [18] generalized the Boltzmann equation to account for particles obeying the BE-FD statistics. For all three statistics the scattering by collisions is sufficiently well described by the Bhatnagar-Gross-Krook (BGK) term [19,20] and the LBM is essentially a numerical implementation of the Boltzmann-BGK equation [21]. Quantum [17,22] and classical particles under thermal gradients [23] have been treated by the LBM in the context of the DHP, which renders to them a very restrictive window of convergence since their EDFs are expanded around the Gaussian function. We show here that significant improvement in convergence of the LBM, and therefore usefulness in its practical descriptions, are obtained if the EDF is expanded near to itself, for a shifted argument, which leads to the new set of \( D \)-dimensional polynomials proposed in this letter. The new polynomials are orthonormal under a weight given by the EDF itself, whereas the DHP is fixed to the Gaussian weight. The isothermal MB LBM is convergent for a small Mach number (\( Ma \approx u/c_r \), \( u \) is the displacement velocity and \( c_r \approx \sqrt{\text{Kn}T_0/m} \) is essentially the speed of sound at temperature \( T_0 \)), whereas the present LBM is convergent for small \( u/c_0 \).

The EDF depends explicitly on the position, \( x \), through the local macroscopic parameters, such as the density \( \rho(x) \) (or the chemical potential \( \mu(x) \)), the macroscopic (displacement) velocity \( u(x) \), and the temperature \( \theta(x) \). The FD (+) and the BE (−) EDFs correspond to \( f_{FD/BE} = |\exp(-\mu/\theta)\exp(\xi/2\theta)|^{-1} \), and the MB is \( f_{MB} = \rho_0 \exp(-\xi^2/2\theta)/(2\pi \theta)^{D/2} \), where \( \rho_0 \) is a dimensionless constant. All variables are defined as dimensionless \( (m = k_B = e = h = 1) \) by means of the scale set by \( T_r \), which fixes \( c_r \). The Chapman-Enskog analysis applies [17], which means that the first three moments are either computable from the non-equilibrium distribution function or from the known EDF [24]. The first three moments are given by \( \rho \equiv \int d^D \xi f_{eq}(\xi - u) \), \( \rho u = \int d^D \xi \xi f_{eq}(\xi - u) \) and \( D\rho\theta = \int d^D \xi (\xi - u)^2 f_{eq}(\xi - u) \), where the third moment is the internal energy, defined through the pseudo-temperature [17], which in the classical case becomes the temperature, \( \theta = \theta \).

Generalized polynomials in \( D \) dimensions. — Consider the \( D \)-dimensional space of the microscopic velocity, \( \xi \equiv (\xi_1, \xi_2, \cdots, \xi_D) \), endowed with a weight function that can be, for instance, any of the three EDFs previously discussed: \( \omega = (f_{FD}, f_{BE}, f_{MB}) \). We claim here the existence of a set of orthonormal polynomials \( P_{i_1 \cdots i_N}(\xi) \), such that

\[
\int d^D \xi \omega(\xi) P_{i_1 \cdots i_N}(\xi) P_{j_1 \cdots j_M}(\xi) = \delta_{NM} \delta_{i_1 \cdots i_N j_1 \cdots j_M},
\]

where \( \omega(\xi) = f_{eq}(\xi, u = 0) \). The DHP correspond to the Gaussian function \( \omega(\xi) = \exp(-\xi^2/2)/(2\pi)^{D/2} \). In fact the existence of the generalised polynomials only relies on some general properties of the weight function, such as the dependence on \( \xi \equiv (\xi) \), which makes it become equal to zero at extremely high microscopic velocities, \( \omega(\xi) \to 0 \) for \( \xi \to \infty \), such that the integrals \( I_N \) given below, are well defined,

\[
\int d^D \xi \omega(\xi) \xi_{i_1} \cdots \xi_{i_N} = I_N \delta_{i_1 \cdots i_N}.
\]

By symmetry it holds that \( I_N = 0 \) for \( N \) odd. We introduce the following tensors which are sums of products of Kronecker’s delta function \( (\delta_{ij} = 1 \text{ for } i = j \text{ and } 0 \text{ for } i \neq j) \), namely, \( \delta_{i_1 \cdots i_N | j_1 \cdots j_N} = \delta_{i_1 j_1} \cdots \delta_{i_N j_N} + \text{all permutations of } j\text{s and } i\text{s} \), and \( \delta_{i_1 \cdots i_N j_1 \cdots j_N} = \delta_{i_1 j_1} \cdots \delta_{i_N j_N} + \text{all permutations. Thus, they contain } N! \text{ and } (2N)! \text{ terms, respectively. Using the aforementioned symmetries the } I_{2N} \text{ are given by}

\[
I_{2N} = \frac{\pi^{D/2}}{2^{N-1} \Gamma(N + \frac{D}{2})} \int_0^{\infty} d\xi \omega(\xi) \xi^{2N+D-1}.
\]

A direct consequence of eqs. (1) and (2) is that the moments are given by \( \rho = I_0 = I_{2/0} \). Like the DHP the new polynomials \( P_{i_1 \cdots i_N}(\xi) \) are symmetrical in the indices \( i_1 \cdots i_N \), have the parity property \( P_{i_1 \cdots i_N}(-\xi_{i_1}, \cdots, -\xi_{i_N}) = (-1)^N P_{i_1 \cdots i_N}(\xi_{i_1}, \cdots, \xi_{i_N}) \) and are tensors in Euclidean space expressed in terms of the vector components \( \xi_i \) and of \( \delta_{ij} \). However, they have a new property not present in the DHP, namely, they are of \( N\)-th order in \( \xi \). This is an important feature that shows that DHP are a sub-class of the new polynomials and not vice versa. The first four ones are given by

\[
P_0(\xi) = c_0,
\]
\[ \mathcal{P}_{i_1}(\xi) = c_1 \xi_{i_1}, \]  
\[ \mathcal{P}_{i_2}(\xi) = c_2 \xi_{i_2} + (\bar{c}_2 \xi^2 + \bar{c}_3 \xi^3 + \bar{c}_4 \xi^4 + \bar{c}_5 \xi^5) \delta_{i_2,i_2}, \]  
\[ \mathcal{P}_{i_3,i_1}(\xi) = c_3 \xi_{i_3} \xi_{i_1} + (\bar{c}_3 \xi^2 + \bar{c}_3 \xi^3) (\xi_{i_3} \delta_{i_2,i_2} + \bar{c}_4 \xi_{i_3} \delta_{i_2,i_2}), \]  
\[ \mathcal{P}_{i_3,i_2,i_1}(\xi) = c_4 \xi_{i_3} \xi_{i_2} \xi_{i_1} + (\bar{c}_4 \xi^2 + \bar{c}_4 \xi^3 + \bar{c}_5 \xi^4 + \bar{c}_5 \xi^5) \delta_{i_3,i_2,i_1} + (\bar{d}_4 \xi^4 + \bar{d}_4 \xi^5 + \bar{d}_4 \xi^6) \delta_{i_3,i_2,i_1}. \]

All the coefficients are solely functions of the integrals 
\[ I_{2N} = c_K = 1/\sqrt{2K} \]  
for \( K = 0, 1, 2, 3, \) and 4, and \( c_K = -c_K (I_{2K-2}/I_{2K-4}) \Delta_{2K-2} K \), for \( K = 1, 2, 3, \) and 4. We define for \( L \) even, 
\[ \Delta_l^2 \equiv 2/([D + L] - J_L (D + L - 2)) \]  
and \( J_L \equiv I_{l/2}^2 + I_{l/2 - 1}^2 \). The remaining coefficients are 
\[ d_4^2 = \frac{8\Delta_2^4}{\Delta_1} \]  
\[ d_4' = \frac{d_4}{D + 2} + c_4 \frac{[D - 2 (D + 2) \Delta_6]}{D + 2 (D + 4)}, \]
where \( \Delta_l \equiv 2I_{l/2}I_{l/2 - 1} / \Delta_l^2 \).

The advantages of the new polynomials over the DHP are clearly seen in the above expression: 
\[ f^{(eq)}(\xi - \mu) = \omega(\xi) \sum_{N=0}^{K} \frac{1}{N!} A_{i_3 i_2 \cdots i_N}(\mu) \mathcal{P}_{i_3 i_2 \cdots i_N}(\xi), \]
where 
\[ A_{i_3 i_2 \cdots i_N}(\mu) = \int d^D \xi f^{(eq)}(\xi - \mu) \mathcal{P}_{i_3 i_2 \cdots i_N}(\xi). \]
such orders, just demanding a small ratio $u/c_0$. Recall that a distinct choice of weight can render coefficients that do not necessarily vanish for $u = 0$, and so, they have other parameters that control their smallness. This is the case of the thermal LBM developed over the Gaussian weight, whose coefficients also depend on the temperature deviation [17,23] from a reference value, $\theta = -1$.

The generalised polynomials make the EDF a function of powers of the ratio $u/c_0$ instead of $u/c$, but notice that up to this point both $u$ and $\xi$ are normalized by $c$. A glance into this change of scale is provided by looking at the highest-order term in the velocities of the polynomials, $P_{i_1i_2\ldots i_N}(\xi) = (1/\sqrt{J_{2N}})\xi_i\xi_{i_2}\ldots\xi_{i_N} + \ldots$, and the coefficients, $A_{i_1i_2\ldots i_N}(u) = (I_0/\sqrt{J_{2N}})u_{i_1}u_{i_2}\ldots u_{i_N} + \ldots$. The presence of the $I_{2N}$ introduces the scale $c_0 = (J_{2N})^{1/2N}$, and we define $\xi' = \xi/c_0$ and $u' = u/c_0$ such that $P_{i_1i_2\ldots i_N}(\xi) = \xi'_i\xi'_{i_2}\ldots\xi'_{i_N} + \ldots$, and $A_{i_1i_2\ldots i_N}(u) = I_0u'_{i_1}u'_{i_2}\ldots u'_{i_N} + \ldots$. Consequently $c_r$ is no longer present, as can be checked, for instance, in the Sommerfeld limit of the FD weight, eq. (12), since $c_0 \sim \sqrt{\tau}$ and because $\mu$ is also normalized by $c_r^2$. The overall result is that the chemical potential sets the new velocity scale.

The Gaussian and the new quadratures. – The Gaussian quadrature provides a way to calculate the integral of a function as a sum over some of its values at a set of points $\alpha$ multiplied by pre-determined weights $w_\alpha$. We claim here that the Gaussian quadrature holds for $\omega(\xi) = f(\xi)(\xi, u = 0)$, such that $\int d^D\xi\omega(\xi)g(\xi) = \sum_\alpha w_\alpha g_\alpha$, $g_\alpha \equiv g(\xi_\alpha)$. Thus, eqs. (3) turn into the following relations:

$$\sum_\alpha w_\alpha \xi_{\alpha i_1}\cdots\xi_{\alpha i_N} = I_N \delta_{i_1\cdots i_N}, \quad (21)$$

such that $I_N = 0$ for $N$ odd. The passage from continuous to discrete consists in determining lattices, namely the sets of $\xi_{\alpha i_1}$ and $w_\alpha$, that satisfy eqs. (21) once known the integrals $I_{2N}$ of eqs. (2). In the present approach the weights become function of the above integrals, $w_\alpha(I_{2N})$, and must be updated at each time step of the evolution procedure.

The normalization of the velocities changes from $c_r$ to $c_0$ once the lattice of geometrical velocities, defined by the set of $\alpha$ vectors $e_\alpha \equiv \xi_\alpha/c_0$, is introduced, to solve eqs. (21). The $e_\alpha$ form a basis that generates an array of regularly spaced points in real space while the lattice of vectors $\xi_\alpha$ does not, and so, it must be locally adjusted by $c_0$. Hereafter we restrict our study to the $N = 3$ order in the EDF of eq. (13) which renders the Navier-Stokes equation from the Chapman-Enskog analysis of the Boltzmann-BGK equation [17]. Therefore, as examples, we consider the following two lattices. The $d1v3$ ($D = 1$) lattice contains only three velocities, $e_0 = 0$, $e_{\pm 1} = \pm 1$ and the associated weights are $w_0 = I_0(1 - J_3/3)$ and $w_{\pm 1} = I_0J_3/6$. The lattice $d2v9$ ($D = 2$) has its geometrical velocities on the sides and diagonals of a square, namely, $e_\alpha, \alpha = 0, \ldots, 8$: $e_0 = (0, 0)$, $e_{\text{long}} = [(1, 1), (1, -1), (-1, 1), (1, -1)]$ and $e_{\text{short}} = [(1, 0), (0, 1), (-1, 0), (0, 1)]$. The corresponding weights are $w_0 = I_0(1 - 5J_9/9)$, $w_{\pm 1} = I_0J_3/36$ and $w_{\pm 1} = I_0J_3/9$, associated to the center, long and short vectors, respectively. For both lattices $c_0 = \sqrt{3}I_1/I_2$. Therefore the $N = 3$ EDF,

$$f^{(eq)} = w_\alpha \left(1 + \frac{I_0}{I_2} \xi_\alpha \cdot u + \frac{I_0}{2I_4} \left(\xi_\alpha \cdot u\right)^2 + \frac{I_0}{2I_4} \frac{\Delta_2^2 u^2}{2} + \frac{1}{6} \frac{I_0}{I_6} \left(\xi_\alpha \cdot u\right)^2 \right),$$

becomes, in the geometrical space,

$$f^{(eq)} = w_\alpha \left(1 + \frac{3}{2} J_4 e_\alpha \cdot u_{\tau} + \frac{9}{2} J_4 e_{\alpha} \cdot u_{\tau} \right)$$

$$+ \frac{9}{4} \left(\frac{\Delta_2^2 - 1}{J_4 I_2} \right) u_{\gamma}^2 e_{\gamma}^2 + \frac{3}{2} I_4 \Delta_2^2 u_{\tau}^2 + \frac{3}{2} J_4 \left(\frac{\Delta_2^2}{J_4 I_2} - 1\right) u_{\gamma}^2 e_{\gamma}^2 + 3 J_4 \left(\frac{\Delta_2^2}{J_4 I_2} - 1\right) u_{\gamma}^2 e_{\gamma}^2 + 3 J_4 \left(\frac{\Delta_2^2}{J_4 I_2} - 1\right) u_{\gamma}^2 e_{\gamma}^2 \right),$$

(22)

The lattice Boltzmann-BGK equation becomes [26]

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

(23)

where $\tau$ is the relaxation time. In conclusion $c_0$ has become the scale velocity in replacement of $c_r$ for the two lattices considered above. Updates are done in the density, which is equivalent to $I_0$, and in the normalized velocity $u_0$.

$$I_0 = \sum_\alpha f_\alpha e_\alpha \quad \text{and} \quad u_0 \equiv \frac{u}{c_0} = \frac{1}{I_0} \sum_\alpha f_\alpha e_\alpha. \quad (24)$$

Numerical simulations for electrons in metals in one and two dimensions. – Here we apply for fermions (electrons in metals) the present LBM based on the new $D$-dimensional polynomials. Performing the so-called Chapman-Enskog analysis [17] we derive the macroscopic hydrodynamic equations for the semiclassical fluid, whose continuity and Navier-Stokes equations are $\partial I_0/\partial t + \partial(I_0 u^i)/\partial x^j = 0$ and

$$\frac{\partial}{\partial t} \left(I_0 u^i\right) + \frac{\partial}{\partial x^j} \left[ I_0 \left( \frac{I_2}{I_0} \delta^{ij} + u^i u^j \right) \right] - \frac{\partial}{\partial x^j} \sigma^{ij} = 0, \quad (25)$$

respectively. The dynamic viscosity is $\eta = I_3 \tau (1 - \Delta_3^2)$. The viscosity stress tensor, $\sigma^{ij} = \eta \left( \frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i} - \frac{2}{D} \delta^{ij} \frac{\partial u}{\partial x} \right)$,
vanishes for $D = 1$, and so the Navier-Stokes equation reduces to the Euler equation [17]. Thus, the $D = 1$ semiclassical fluid is not dissipative for any $\tau$.

For $D = 1$ we make a direct comparison between a known solution of the Euler equation in the case of a stepwise initial condition, the so-called Riemann problem [27], and our numerical solution of the one-dimensional Boltzmann equation. We take zero temperature ($\theta = 0$) at eq. (12). This renders $I_{0} = (2\pi \mu) \frac{1}{\Gamma(\frac{D}{2} + 1)}$, $J_{N} = 1 + 2/(N + D)$ and $\Delta^{2}_{N} = (D + N)/2$. Local changes in $\rho$ and $u$ are only possible due to local variations in the chemical potential. We use the two lattices, $d1v3$ ($w_{1} = 7I_{0}/12$ and $w_{1} = 5I_{0}/24$) and $d2v9$ ($w_{0} = 3I_{0}/5$, $w_{1} = I_{0}/30$ and $w_{2} = 2I_{0}/15$). In this case the weights are constant in all lattice points with a remaining multiplicative density played by $I_{0}$ such as in the known LBM method [28]. The velocity scale, $v_{0} = \sqrt{6\mu/(D + 4)}$, is essentially the Fermi velocity. For both lattices we find independence of the numerical solution with respect to $\tau$ within a wide range ($\tau = 0.57–0.95$, reduced units). Figure 1 shows the comparison between the obtained $\rho$ 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 ($PV = N_{0} \cdot \frac{\hbar kT}{N_{0}}$, $N_{0} = 2/5$ in 3D). Figure 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 $d2v9$ lattices. Therefore, we allow for an adjustment of $N_{0}$ in the definition of pressure used in the solver of ref. [27] for the Euler equation to obtain agreement between the classical and the semi-classical gas velocities. The solver also leads to agreement in the density of the two gases. For $D = 2$ we simulate a horizontal flow through rigid obstacles randomly placed with $d2v9$, as depicted in fig. 2(a). We show here that Ohm’s law or, equivalently, Darcy’s law [29], work for the semi-classical fluid in a porous media as there is a proportionality between the velocity and the applied force. Figure 2(a) shows the modulus of the velocity field, $|u|$, inside a medium of porosity 0.992, that is, the obstacles take 0.8% of the total number of nodes. The bounce-back boundary conditions are used around the obstacles and the periodic boundary conditions in the borders. Figure 2(b) shows the resulting proportionality between the applied force, defined according to the prescription of ref. [26], and the velocity, which is the average velocity in the direction of the force, $\langle u \rangle$. Figure 2(a) corresponds to the highest force of fig. 2(b).

**Conclusions.** – Semi-classical flows are treated through a LBM based on new polynomials, which are orthonormal in the $D$-dimensional Euclidean space endowed with a weight function defined by the equilibrium distribution function itself. Numerical results show that i) the semi-classical one-dimensional flow (Riemann problem) is described by Euler’s equations, and ii) a two-dimensional conducting stripe with insulating obstacles obeys Darcy’s law [29].
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