From the continuous to the lattice Boltzmann equation: The discretization problem and thermal models

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The velocity discretization is a critical step in deriving the lattice Boltzmann (LBE) from the continuous Boltzmann equation. This problem is considered in the present paper, following an alternative approach and giving the minimal discrete velocity sets in accordance with the order of approximation that is required for the LBE with respect to the continuous Boltzmann equation and with the lattice structure. Considering N to be the order of the polynomial approximation to the Maxwell-Boltzmann equilibrium distribution, it is shown that solving the discretization problem is equivalent to finding the inner product in the discrete space induced by the inner product in the continuous space that preserves the norm and the orthogonality of the Hermite polynomial tensors in the Hilbert space generated by the functions that map the velocity space onto the real numbers space. As a consequence, it is shown that, for each order N of approximation, the even-parity velocity tensors are isotropic up to rank $2N$ in the discrete space. The norm and the orthogonality restrictions lead to space-filling lattices with increased dimensionality when compared with presently known lattices. This problem is discussed in relation with a discretization approach based on a finite set of orthogonal functions in the discrete space. Two-dimensional square lattices intended to be used in thermal problems and their respective equilibrium distributions are presented and discussed.

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I. INTRODUCTION

In accordance with Lallemand and Luo [1], the presently known lattice Boltzmann equation (LBE) has not been able to handle realistic thermal (and fully compressible flow) problems with satisfaction. Simulation of the thermal lattice Boltzmann equation is hampered by numerical instabilities when the local velocity increases.

The first thermal lattice Boltzmann models were introduced in about 1990 and there are several reasons that may be conjectured for their failure in handling nonisothermal flows [1].

Considering the kinetic nature of the LBE, establishing a formal link connecting the LBE to the continuous Boltzmann equation, and enabling the conceptual analysis of this discrete numerical scheme could perhaps shed some light on this question.

Indeed, there are several features that cause the lattice Boltzmann regular-lattice based framework to be far removed from the continuous Boltzmann equation, which would be desirable to be its conceptual support. These features include the particles, collision, and long-range interaction models, and the approach used for the time and the velocity space discretization.

Historically, the LBE was introduced by McNamara and Zanetti [2], replacing the Boolean variables in the discrete collision-propagation equations by their *ensemble* averages. Higuera and Jimenez [3] proposed a linearization of the collision term derived from the Boolean models, recognizing that this full form was unnecessarily complex when the main purpose was to retrieve the hydrodynamic equations. Following this line of reasoning, Chen *et al.* [4] suggested replacing the collision term by a single relaxation-time term, followed by Qian *et al.* [5] and Chen *et al.* [6], who introduced a model based on the celebrated kinetic-theory idea of Bhatnagar, Gross, and Krook (BGK) [7], but adding rest particles and retrieving the correct incompressible Navier-Stokes equations, with third-order nonphysical terms in the local speed, u.

The BGK collision term describes the relaxation of the distribution function to an equilibrium distribution. This discrete equilibrium distribution was settled by writing it as a second-order polynomial expansion in the particle velocity $\boldsymbol{c}_i$, with parameters adjusted to retrieve the mass density, the local velocity, and the momentum flux equilibrium moments, which are necessary conditions for satisfying the Navier-Stokes equations.

Thermal lattice BGK schemes included higher-order terms in the equilibrium distribution function [8,9], requiring one to increase the lattice dimensionality [8–10], i.e., the number of vectors in the finite and discrete velocity set $\{\boldsymbol{c}_i, i=0,\ldots,b\}$.

In thermal problems, the BGK single relaxation-time collision term restricts the models to a fixed Prandtl number. The correct description of fluids and fluid flow requires multiple relaxation-time models (MRT). A two-parameter model was introduced by He *et al.* [11] using two sets of distributions for the particle number density and the thermodynamic internal energy, coupled through a viscous dissipation term. Full MRT models were first introduced in the LBE framework by d'Humières [12,13] by modifying the collision step, considering it to be given by the relaxation to the equilibrium of a set of nonpreserved kinetic moments.

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Most lattice Boltzmann simulations are based on an explicit numerical scheme, although some lattice BGK models have been simulated with implicit numerical schemes [14,15] or LBE modified explicit numerical schemes [11], increasing by 1 the order of the time step errors.

With a few exceptions, in all the above works there is no formal link connecting LBE to the continuous Boltzmann equation, although the main ideas were based on the kinetic theory fundamentals.

He and Luo [16] have directly derived the LBE from the continuous Boltzmann equation for some widely known lattices (D2Q9, D2Q6, D2Q7, D3Q27) by the discretization of the velocity space, using the Gauss-Hermite and Gauss-Radau quadrature. Unfortunately, excluding the abovementioned lattices, the discrete velocity sets obtained by this kind of quadrature do not generate regular, space-filling, lattices.

Succi [17], referring to He and Luo's work, suggests that establishing the exact nature of the link between the LBE and the continuum kinetic theory could be useful for systematic analysis and for the potential derivation of novel LBE numerical schemes.

The present paper deals with the aspects involved in deriving space-filling lattices that should be suitable for thermohydrodynamic problems. We start from the continuous Boltzmann equation, and the derivation of discrete velocity sets is considered as a quadrature problem, i.e., (a) to find a set of discrete velocities, $\boldsymbol{c}_i$, and weights W_i such that all the desired macroscopic moments are *exactly* retrieved as moments of the discrete equilibrium distribution f_i^{eq}, and (b) to ensure isotropy for the even-parity rank velocity tensors and, consequently, for the fluid transfer properties.

In doing that, two questions must be solved.

The first question is how to avoid the temperature dependence of the particles discrete velocities. This is a common drawback when performing Gauss-Hermite and related quadratures, using the dimensionless particle velocity $\mathcal{C} = c/\sqrt{2k/Tm}$ as the integration variable, and leads to temperature-dependent particle velocities [18]. This problem is solved here by letting the particle velocity, c^2, be free from the temperature T in the exponential part e^{-c^2} of the Maxwell-Boltzmann (MB) distribution, and leads to writing the equilibrium distribution as a Taylor expansion in terms of the temperature deviation Θ. A similar approach is presented in [19].

The second question is how to derive *space-filling* lattices from the quadrature of the continuous Boltzmann equation.

Shan and He [20] showed that by discretizing the Boltzmann-BGK equation at a set of velocity vectors that correspond to the nodes of a Gauss-Hermite quadrature in the velocity space, the Boltzmann equation is effectively projected on a subspace spanned by the leading Hermite polynomials. Nevertheless, the quadrature problem leading to a minimum number of nodes for a given degree of accuracy was considered by these authors as a still unsolved problem. In addition, these authors mention the use of alternative numerical schemes such as the finite differences method, considering that these nodes do not, in general, coincide with the vertices of a regular lattice. More recently, Pavlo *et al.* [18] proposed a temperature-dependent velocity model based on an octagonal lattice, which is not space-filling, but ensures the isotropy of sixth-rank velocity tensors.

Given that the velocity discretization is a critical step in deriving lattice Boltzmann equations, this problem is considered in the present paper, following an alternative approach and giving the minimal discrete velocity sets in accordance with the order of approximation that is required for the LBE with respect to the continuous Boltzmann equation and with the lattice structure.

Considering N to be the order of the polynomial approximation to the MB equilibrium distribution, it is shown that solving the quadrature problem is *equivalent* to finding the inner product $(f * g)_d$ in the discrete space induced by the inner product $(f * g)_c$ in the continuous space, which preserves the norm and the orthogonality of the Hermite polynomial tensors $\Psi_{\theta,(r_\theta)}$. As a consequence, it is also shown that for each $\theta = 1, \ldots, N$, the 2θ-rank velocity tensors are isotropic in the discrete space.

Two-dimensional square lattices intended to be used in thermal problems and their respective discrete equilibrium distributions are presented and discussed.

Finally, a discretization approach based on a set of orthogonal functions in the discrete space is discussed in detail, in relation with the presently proposed velocity discretization method.

II. THE DISCRETIZATION PROBLEM IN THE LATTICE BOLTZMANN FRAMEWORK

The classical lattice Boltzmann method is based on (i) a regular lattice generated by a space-filling discrete velocity set $\{\boldsymbol{c}_i, i = 0 \ldots, b\}$ and (ii) a discrete form of the Boltzmann equation, with a single or multiple relaxation time collision model and an equilibrium solution.

A Chapman-Enskog analysis of the lattice BGK equation [10] shows that a set of *necessary* conditions for the correct thermohydrodynamic equations to be retrieved is given by assuring that the discrete distributions f_i^{eq} satisfy

$$\langle \varphi_p \rangle^{\mathrm{eq}} = \frac{1}{n_d} \int f^{\mathrm{eq}}(\boldsymbol{c}) \varphi_p(\boldsymbol{c}) d\boldsymbol{c} = \frac{1}{n} \sum_i f_i^{\mathrm{eq}} \varphi_p(\boldsymbol{c}_i) \qquad (1)$$

for $\{\varphi_p = 1, c_\alpha, c_\alpha c_\beta, c_\alpha c_\beta c_\gamma, c^2 c_\alpha c_\beta\}$, where $f^{\mathrm{eq}}(\boldsymbol{c})$ is the MB distribution written in terms of the particle velocity $\boldsymbol{c}$ in the continuous space, n_d is the number density of particles, n is the number of particles per site, and $\langle \varphi_p \rangle^{\mathrm{eq}}$ denotes a macroscopic equilibrium moment of φ_p.

Frequently, in athermal and thermal lattice Boltzmann models (e.g., [9]), the *unknown* discrete equilibrium distributions $f_{i,N}^{\mathrm{eq}}$ for a given order of approximation, N, are derived as *finite* expansions in the particle velocity $\boldsymbol{c}_i$,

$$\frac{f_{i,N}^{\mathrm{eq}}}{n} = A + B_\alpha c_{i\alpha} + D_{\alpha\beta} c_{i\alpha} c_{i\beta} + \cdots + O(N), \qquad (2)$$

with free parameters that are determined considering the symmetries of a previously chosen lattice

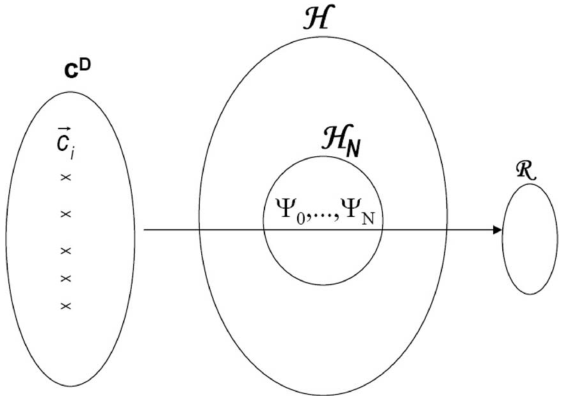

FIG. 1. The Hilbert space and the discretization problem.

$\ell=\{c_i, i=0,\ldots,b\}$ and adjusted to satisfy Eq. (1) for all $\langle\varphi_p\rangle^{eq}$ of interest.

This approach is equivalent to replacing the full MB distribution on the left-hand side of Eq. (1) by a finite expansion in $\boldsymbol{c}$. In this manner, the moments, $A, B_\alpha, D_{\alpha\beta},\ldots$ in Eq. (2) are calculated to fit the MB distribution at each order of approximation and, as a consequence, are dependent on N.

Since we cannot expect to find any relationship between $f^{eq}(\boldsymbol{c}_i)$ and $f^{eq}_{i,N}$, consider now the question of finding the relationship between $f^{eq}_N(\boldsymbol{c})$ and $f^{eq}_{i,N}$ when $\boldsymbol{c}\rightarrow\boldsymbol{c}_i$. Distribution $f^{eq}_N(\boldsymbol{c})$ is the projection of the full MB distribution on the function space spanned by functions $\{1, c_\alpha, c_\alpha c_\beta,\ldots\}$. Given that distributions $f^{eq}_{i,N}$ are only required to retrieve the equilibrium moments, there are no means to assure that $f^{eq}_N(\boldsymbol{c})$ approaches $f^{eq}_{i,N}$ (in fact, a weighted $f^{eq}_{i,N}$) when $\boldsymbol{c}\rightarrow\boldsymbol{c}_i$.

The result is that, although the equilibrium moments are preserved with these finite expansions, the equilibrium distribution $f^{eq}_{i,N}$ has no local identification with the projection $f^{eq}_N(\boldsymbol{c})$ of the full MB distribution on the function space spanned by $\{1, c_\alpha, c_\alpha c_\beta,\ldots\}$. Section IV gives a more detailed discussion about this problem.

In the present work, discretization is considered as a quadrature problem. In this manner, f^{eq}_i is replaced by a weighted f^{eq}, preventing the above drawback.

Let $\mathcal{H}$ be the Hilbert weighted L_2 space generated by functions $f: c^D\rightarrow\mathcal{R}$ that map the D-dimensional continuous velocity space, c^D, onto the real variables space, $\mathcal{R}$ (Fig. 1). Velocity discretization means replacing the entire velocity space c^D by some few velocity vectors. When discretization is considered as a *quadrature* problem, the discrete distributions f^{eq}_i/n on the right-hand side of Eq. (1) must be replaced by $f^{eq}(\boldsymbol{c}_i)/n_d$, i.e., by the value of the MB distribution evaluated at the pole $\boldsymbol{c}_i$ multiplied by a parameter ω_i, which denotes the weight to be attributed to each velocity vector $\boldsymbol{c}_i$ to satisfy the quadrature condition, considering that, for each coordinate axis α, the lattice speeds $c_{i\alpha}$ form a discrete and finite set and the continuous velocity space is continuous and extends to infinity.

In this manner, the discretization restrictions, Eq. (1), are replaced by the following quadrature equations:

$$\langle\varphi_p\rangle^{eq} = \int \frac{f^{eq}(\boldsymbol{c})}{n_d}\varphi_p(\boldsymbol{c})d\boldsymbol{c} = \sum_i \omega_i\left(\frac{2kT}{m}\right)^{D/2}\frac{f^{eq}(\boldsymbol{c}_i)}{n_d}\varphi_p(\boldsymbol{c}_i), \tag{3}$$

where the factor $(2kT/m)^{D/2}$ was introduced to assure ω_i is a dimensionless, real number, since $f^{eq}(\boldsymbol{c})/n_d$ is the number of particles per unit volume of the velocity space.

The role of the integration variable

Considering T to be the local temperature, $\boldsymbol{c}$ the particle velocity, $\boldsymbol{u}$ the macroscopic local velocity, m the mass of each particle, and $\boldsymbol{\mathcal{C}}_f=(\boldsymbol{c}-\boldsymbol{u})/\sqrt{2kT/m}$ the dimensionless peculiar velocity, the Maxwell-Boltzmann equilibrium distribution can be written as

$$f^{eq} = n_d\left(\frac{m}{2\pi kT}\right)^{D/2} e^{-\boldsymbol{\mathcal{C}}_f^2}. \tag{4}$$

Returning to Eq. (3), when performing the quadrature, an integration variable must be chosen. If the dimensionless peculiar velocity, $\boldsymbol{\mathcal{C}}_f$, is chosen as the integration variable,

$$\langle\varphi_p\rangle^{eq} = \frac{1}{\pi^{D/2}}\int e^{-\boldsymbol{\mathcal{C}}_f^2}\varphi_p(\boldsymbol{\mathcal{C}}_f)d\boldsymbol{\mathcal{C}}_f = \sum_{i=0}^{b} W_i\varphi_p(\boldsymbol{\mathcal{C}}_{fi}), \tag{5}$$

where $\boldsymbol{\mathcal{C}}_{fi}$ is a discrete peculiar velocity (a constant vector) dependent, basically, on b and on the kind of quadrature that was performed and

$$W_i = W_i(|\boldsymbol{\mathcal{C}}_{fi}|) = \frac{\omega_i e^{-\boldsymbol{\mathcal{C}}_{fi}^2}}{\pi^{D/2}} \tag{6}$$

are the dimensionless weights to be attributed to each discrete velocity $\boldsymbol{\mathcal{C}}_{fi}$.

For the first kinetic moment, n,

$$\langle 1\rangle = \frac{1}{\pi^{D/2}}\int e^{-\boldsymbol{\mathcal{C}}_f^2}1d\boldsymbol{\mathcal{C}}_f = \sum_{i=0}^{b} W_i 1 = \sum_{i=0}^{b} W_i, \tag{7}$$

resulting in

$$f^{eq}_i = W_i n. \tag{8}$$

This means that the discrete equilibrium distribution does not depend, *explicitly*, on the macroscopic velocity $\boldsymbol{u}$ and on the temperature T. Nevertheless, the temperature and local velocity dependences are included in the particle velocities through

$$\boldsymbol{c}_i = \boldsymbol{u} + \left(\frac{2kT}{m}\right)^{1/2}\boldsymbol{\mathcal{C}}_{fi} = \boldsymbol{c}_i(T,\boldsymbol{u}). \tag{9}$$

In this manner, the *physical* grid, $(\boldsymbol{x},\boldsymbol{c}_i)$, i.e., the *physical* grid points where the particles will be located after each time step, will be time-dependent. Simulation tends to be very cumbersome and, at first glance, boundary conditions will be difficult to satisfy.

Another choice is the dimensionless particle velocity $\mathcal{C}=\boldsymbol{c}/(2kT/m)^{1/2}$. This is the usual choice in LBM and requires us to rewrite the equilibrium distribution as

$$f^{\text{eq}} = n_d\left(\frac{m}{2\pi kT}\right)^{D/2} e^{-\mathcal{C}^2} e^{2\mathcal{U}\cdot\mathcal{C}-\mathcal{U}^2}, \tag{10}$$

where $\mathcal{U}=\boldsymbol{u}/(2kT/m)^{1/2}$ is a dimensionless local velocity and $\mathcal{C}=\boldsymbol{c}/(2kT/m)^{1/2}$. The use of $\mathcal{C}$ as the integration variable instead of $\mathcal{C}_f$ requires us to develop $e^{2\mathcal{U}\cdot\mathcal{C}-\mathcal{C}^2}$ as an infinite series of Hermite polynomial tensors $\Psi_{\theta,(r_\theta)}$ [21], resulting in

$$f^{\text{eq}} = n_d\frac{e^{-\mathcal{C}^2}}{\pi^{D/2}}\left(\frac{m}{2kT}\right)^{D/2}\sum_\theta a^{\text{eq}}_{\theta,(r_\theta)}(\mathcal{U})\Psi_{\theta,(r_\theta)}(\mathcal{C}), \tag{11}$$

where (r_θ) is a sequence of indexes $r_1, r_2, \ldots, r_\theta$ (repeated indexes mean summation),

$$\Psi_0 = 1, \tag{12}$$

$$\Psi_{1,\alpha} = 2C_\alpha, \tag{13}$$

$$\Psi_{2,\alpha\beta} = 2\left(C_\alpha C_\beta - \frac{1}{2}\delta_{\alpha\beta}\right), \tag{14}$$

$$\Psi_{3,\alpha\beta\gamma} = \frac{4}{3}\left[C_\alpha C_\beta C_\gamma - \frac{1}{2}(C_\alpha\delta_{\beta\gamma} + C_\beta\delta_{\alpha\gamma} + C_\gamma\delta_{\alpha\beta})\right], \tag{15}$$

$$\Psi_{4,\alpha\beta\gamma\delta} = \frac{2}{3}\left[C_\alpha C_\beta C_\gamma C_\delta - \frac{1}{2}(C_\alpha C_\beta\delta_{\gamma\delta} + C_\alpha C_\gamma\delta_{\beta\delta} + C_\alpha C_\delta\delta_{\beta\gamma} + C_\beta C_\gamma\delta_{\alpha\delta} + C_\beta C_\delta\delta_{\alpha\gamma} + C_\gamma C_\delta\delta_{\alpha\beta}) + \frac{1}{4}\Delta_{\alpha\beta\gamma\delta}\right], \tag{16}$$

and so on. Tensor Δ is defined as $\Delta_{\alpha\beta\gamma\delta}=\delta_{\alpha\beta}\delta_{\gamma\delta}+\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma}$. The above tensors are orthogonal in the Hilbert space $\mathcal{H}$, with respect to the inner product

$$(h * g)_c = \frac{1}{\pi^{D/2}}\int e^{-\mathcal{C}^2} hg\, d\mathcal{C}, \tag{17}$$

and symmetric with respect to any index permutation.

The coefficients $a^{\text{eq}}_{\theta,(r_\theta)}$ in Eq. (11) are the macroscopic moments $a^{\text{eq}}_0=1$, $a^{\text{eq}}_{1,\alpha}=U_\alpha$, $a^{\text{eq}}_{2,\alpha\beta}=U_\alpha U_\beta$, $a^{\text{eq}}_{3,\alpha\beta\gamma}=U_\alpha U_\beta U_\gamma$, $a^{\text{eq}}_{4,\alpha\beta\gamma\delta}=U_\alpha U_\beta U_\gamma U_\delta$, and so on.

Second-order approximations to the MB distribution are widely used in LBM athermal simulation, but, as seen in the beginning of the present section, thermohydrodynamics require fourth-order approximations for the equilibrium distribution. Consider a given Nth-order approximation to the MB distribution,

$$f^{\text{eq}}_N = n_d\frac{e^{-C^2}}{\pi^{D/2}}\left(\frac{m}{2kT}\right)^{D/2}\sum_{\theta=0}^{N} a^{\text{eq}}_{\theta,(r_\theta)}(\mathcal{U})\Psi_{\theta,(r_\theta)}(\mathcal{C}), \tag{18}$$

which can be viewed as an Nth-order Taylor expansion of the full MB distribution, in fact $f^{\text{eq}}e^{C^2}$ (up to some local factors), on the local velocity $\vec{U}$, with errors $O(U^{N+1})$.

After quadrature, the equilibrium distribution becomes

$$f^{\text{eq}}_{i,N} = W_i n\sum_{\theta=0}^{N} a^{\text{eq}}_{\theta,(r_\theta)}(\mathcal{U})\Psi_{\theta,(r_\theta)}(\mathcal{C}_i), \tag{19}$$

where, as above, the constant velocity vectors $\mathcal{C}_i$ are dependent on b and on the kind of quadrature that was performed.

The resulting $\boldsymbol{c}_i$ remains temperature-dependent, through

$$\boldsymbol{c}_i = \left(\frac{2kT}{m}\right)^{1/2}\mathcal{C}_i = \boldsymbol{c}_i(T), \tag{20}$$

which means that after each time step, particles will be propagated to intermediate positions between next-neighboring sites, requiring us to write allocation rules that preserve, locally, the mass, momentum, and energy of the particles packet [18].

III. QUADRATURE BASED ON PRESCRIBED ABSCISSAS

Avoiding the $\boldsymbol{c}_i$ temperature dependence requires us to consider the particle velocity $\boldsymbol{c}$ as the integrating variable when performing the quadrature, i.e., to let c^2 be free from T in the exponential part e^{-C^2} of the equilibrium distribution. This can be accomplished by writing

$$e^{-(c-u)^2/(2kT/m)} = (e^{-C^2_{fo}})^{T_0/T}, \tag{21}$$

where T_0 is a reference (and constant) temperature and $\mathcal{C}_{fo}=(\boldsymbol{c}-\boldsymbol{u})/(2kT_0/m)^{1/2}$ is a new dimensionless peculiar velocity referred to the temperature T_o.

When T is near T_0, i.e., when the departures from thermal equilibrium are small, the above expression may be developed in a Taylor series around $T/T_o=1$. Considering $\Theta=T/T_o-1$ to be the temperature deviation, this development gives

$$(e^{-C^2_{fo}})^{T_0/T} = e^{-C^2_{fo}}\left[1 + C^2_{fo}\Theta + \frac{1}{2}C^2_{fo}(C^2_{fo}-2)\Theta^2 + \cdots\right], \tag{22}$$

which terms are increasing powers of C^2_{fo}.

In this way,

$$f^{\text{eq}} = n_d\left(\frac{T_0}{T}\right)^{D/2}\left[1 + C^2_{fo}\Theta + \frac{1}{2}C^2_{fo}(C^2_{fo}-2)\Theta^2 + \cdots\right] \times\frac{1}{\pi^{D/2}}\left(\frac{m}{2kT_0}\right)^{D/2} \times e^{-C^2_o}\sum_\theta a^{\text{eq}}_{\theta,(r_\theta)}(\mathcal{U}_0)\Psi_{\theta,(r_\theta)}(\mathcal{C}_{0,i}), \tag{23}$$

where $\mathcal{U}_0=\boldsymbol{u}/(2kT_0/m)^{1/2}$.

When the term $(T_0/T)^{D/2}$ is also developed in a Taylor series in terms of the temperature deviation Θ, replacing $\mathcal{C}_{fo}=\mathcal{C}_o-\mathcal{U}_0$, Eq. (23) can be written, after mutiplying the several terms and reorganizing the resulting expression in terms of increasing order of the Hermite polynomials $\Psi_{\theta,(r_\theta)}$, as

$$f^{\rm eq} = \frac{1}{\pi^{D/2}}\left(\frac{m}{2kT_0}\right)^{D/2} e^{-C_0^2}\sum_\theta a^{\rm eq}_{\theta,(r_\theta)}(n_d,\boldsymbol{\mathcal{U}}_0,\Theta)\Psi_{\theta,(r_\theta)}(\boldsymbol{\mathcal{C}}_o), \tag{24}$$

where

$$a_0^{\rm eq} = n_d, \tag{25}$$

$$a^{\rm eq}_{1,\alpha} = n_d\mathcal{U}_{0,\alpha}, \tag{26}$$

$$a^{\rm eq}_{2,\alpha\beta} = n_d\mathcal{U}_{0,\alpha}\mathcal{U}_{0,\beta} + \frac{1}{2}n_d\Theta\,\delta_{\alpha\beta}, \tag{27}$$

$$a^{\rm eq}_{3,\alpha\beta\gamma} = n_d\mathcal{U}_{0,\alpha}\mathcal{U}_{0,\beta}\mathcal{U}_{0,\gamma} + \frac{3}{2}n_d\Theta\mathcal{U}_{0,\gamma}\delta_{\alpha\beta}, \tag{28}$$

$$a^{\rm eq}_{4,\alpha\beta\gamma\delta} = n_d\mathcal{U}_{0,\alpha}\mathcal{U}_{0,\beta}\mathcal{U}_{0,\gamma}\mathcal{U}_{0,\delta} + 3n_d\Theta\mathcal{U}_{0,\alpha}\mathcal{U}_{0,\beta}\delta_{\gamma\delta} + \frac{3}{4}n_d\Theta^2\delta_{\alpha\beta}\delta_{\gamma\delta}, \tag{29}$$

related, respectively, to following macroscopic properties at equilibrium: the number density of particles n_d, the local momentum $n_dU_{0,\alpha}$, the momentum flux $\Pi^{\rm eq}_{\alpha\beta}$, the energy flux $e^{\rm eq}_{\alpha\beta\gamma}$, and a hyperflux of momentum, $\Xi^{\rm eq}_{\alpha\beta\gamma\delta}$.

Since each $\varphi_p(\boldsymbol{c})$ is a p-order monomial tensor in $\boldsymbol{c}$, functions $\Psi_{\theta,(r_\theta)}$ can be written as

$$\Psi_{\theta,(r_\theta)} = \sum_{\eta=0}^{\theta} a^\theta_{\eta,(s_\eta)}\varphi_\eta. \tag{30}$$

In this manner, for a given order θ, after multiplying Eq. (3) by the constants $a^\theta_{\eta,(s_\eta)}$, $\eta=0,\ldots,\theta$ and adding the resulting equations, the quadrature equation, Eq. (3), can be rewritten in terms of quadrature equations for each $\Psi_{\theta,(r_\theta)}$ in the orthogonal basis of $\mathcal{H}$,

$$\int \frac{f^{\rm eq}(\boldsymbol{c})}{n_d}\Psi_{\theta,(r_\theta)}d\boldsymbol{c} = \sum_i \omega_i\left(\frac{2kT_0}{m}\right)^{D/2}\frac{f^{\rm eq}(\boldsymbol{c}_i)}{n_d}\Psi_{\theta,(r_\theta)}(\boldsymbol{c}_i). \tag{31}$$

Using the development, Eq. (24),

$$\sum_\eta a^{\rm eq}_{\eta,(s_\eta)}\frac{1}{\pi^{D/2}}\int e^{-C_0^2}\Psi_{\eta,(s_\eta)}(\boldsymbol{\mathcal{C}}_o)\Psi_{\theta,(r_\theta)}(\boldsymbol{\mathcal{C}}_o)d\boldsymbol{\mathcal{C}}_o = \sum_\eta a^{\rm eq}_{\eta,(s_\eta)}\sum_i W_i\Psi_{\theta,(r_\theta)}(\boldsymbol{\mathcal{C}}_{o,i})\Psi_{\eta,(s_\eta)}(\boldsymbol{\mathcal{C}}_{o,i}), \tag{32}$$

where

$$W_i = W_i(|\boldsymbol{\mathcal{C}}_{0i}|) = \frac{1}{\pi^{D/2}}\omega_i e^{-\boldsymbol{\mathcal{C}}_{0i}^2}. \tag{33}$$

Since each $a^{\rm eq}_{\eta,(s_\eta)}$ is an independent equilibrium moment, Eq. (32) gives

$$\sum_i W_i\Psi_{\theta,(r_\theta)}(\boldsymbol{\mathcal{C}}_{o,i})\Psi_{\eta,(s_\eta)}(\boldsymbol{\mathcal{C}}_{o,i}) = \frac{1}{\pi^{D/2}}\int e^{-C_0^2}\Psi_{\eta,(s_\eta)}(\boldsymbol{\mathcal{C}}_o)\Psi_{\theta,(r_\theta)}(\boldsymbol{\mathcal{C}}_o)d\boldsymbol{\mathcal{C}}_o. \tag{34}$$

Consider the inner products in the continuous and discrete space, respectively;

$$(f*g)_c \equiv \frac{1}{\pi^{D/2}}\int e^{-C_0^2}fg\,d\boldsymbol{\mathcal{C}}_0, \tag{35}$$

$$(f*g)_d \equiv \sum_i W_i f(\boldsymbol{\mathcal{C}}_{o,i})g(\boldsymbol{\mathcal{C}}_{o,i}), \tag{36}$$

and their induced norms

$$\|f\|_c^2 \equiv \frac{1}{\pi^{D/2}}\int e^{-C_0^2}f^2 d\boldsymbol{\mathcal{C}}_0, \tag{37}$$

$$\|f\|_d^2 \equiv \sum_i W_i f^2(\boldsymbol{\mathcal{C}}_{o,i}). \tag{38}$$

Since functions $\Psi_{\theta,(r_\theta)}(\boldsymbol{\mathcal{C}}_o)$ are orthogonal in the continuous space with respect to the inner product Eq. (35), Eq. (34) requires the orthogonality of $\Psi_{\theta,(r_\theta)}(\boldsymbol{\mathcal{C}}_{o,i})$ in the discrete space, with respect to the inner product Eq. (36). In addition, Eq. (34) requires the norm preservation of $\Psi_{\theta,(r_\theta)}$,

$$\sum_i W_i\Psi^2_{\theta,(r_\theta)}(\boldsymbol{\mathcal{C}}_{o,i}) = \frac{1}{\pi^{D/2}}\int e^{-C_0^2}\Psi^2_{\theta,(r_\theta)}(\boldsymbol{\mathcal{C}}_o)d\boldsymbol{\mathcal{C}}_o. \tag{39}$$

In this manner, the still unknown weights W_i and the discrete velocities $\boldsymbol{\mathcal{C}}_{o,i}$ must be chosen in such a manner that the orthogonality of the Hermite polynomial tensors $\Psi_{\theta,(r_\theta)}$ is assured in the discrete space and satisfying the norm preservation equation, Eq. (39).

In Appendix A, it is shown that the norm-preservation equation warrants the orthogonality of $\Psi_{\theta,(r_\theta)}(\boldsymbol{\mathcal{C}}_{o,i})$ with respect to the inner product, Eq. (36), when the discrete velocity space is a Bravais lattice.

The above conclusion is very important because it shows that the norm-preservation equation warrants the orthogonality of $\Psi_{\theta,(r_\theta)}(\boldsymbol{\mathcal{C}}_{o,i})$ in the discrete space, with respect to the inner product, Eq. (36). This reduces our discretization problem to find the weights W_i and the poles $\boldsymbol{\mathcal{C}}_{oi}$ satisfying, solely, the norm restrictions, Eq. (39).

Let $\mathcal{H}_N$ be the subspace of $\mathcal{H}$ generated by the first Hermite polynomials with order $s\leqslant N$ and $f_N^{\rm eq}(c)$ be the projection of the MB distribution, $f^{\rm eq}(c)$, on this subspace. Function $f_N^{\rm eq}e^{\boldsymbol{\mathcal{C}}_0^2}$ is an Nth -order $\boldsymbol{c}$-polynomial tensor and $f_N^{\rm eq}$ can be written as

$$f_N^{\rm eq} = \frac{e^{-C_0^2}}{\pi^{D/2}}\sum_{\theta=0}^{N} a^{{\rm eq},N}_{\theta,(r_\theta)}(n_d,\boldsymbol{\mathcal{U}}_0,\Theta)\Psi_{\theta,(r_\theta)}. \tag{40}$$

Due to the orthogonality and completeness of $\Psi_{\theta,(r_\theta)}$,

$$a^{{\rm eq},N}_{\theta,(r_\theta)}(n_d,\boldsymbol{\mathcal{U}}_0,\Theta) = a^{\rm eq}_{\theta,(r_\theta)}(n_d,\boldsymbol{\mathcal{U}}_0,\Theta) \tag{41}$$

for $\theta\leqslant N$, meaning that the moments $a^{\rm eq}_{\theta,(r_\theta)}$ of the *full* MB distribution are *preserved* when calculated in $\mathcal{H}_N$ with the approximation f_N^{eq}. Although this is a trivial consequence of the functional structure of the Hilbert space $\mathcal{H}$, the above equation is of great importance in lattice Boltzmann theory and means that an Nth-order approximation to the equilibrium distribution is required when Nth-order macroscopic equilibrium moments are to be correctly described in LBM. In addition, since LBM is a kinetic method based on a special discrete form of the Boltzmann equation, the degree of accuracy of the solution will be limited by N.

The above considerations also mean that if real positive weights W_i and velocities $\boldsymbol{\mathcal{C}}_{oi}$ can be found satisfying the norm-preservation conditions, the 2θ-rank velocity tensors

$$\Lambda_{(r_\theta),(s_\theta)} = \sum_i W_i C_{0,i,r_0} \cdots C_{0,i,r_\theta} C_{0,i,s_0} \cdots C_{0,i,s_\theta} \qquad (42)$$

are isotropic for all $\theta=1,\ldots,N$. This property follows directly from the isotropy of these velocity tensors in the continuous space. Indeed, each function $C_{0,i,r_0}\cdots C_{0,i,r_\theta}$ can be written in terms of a linear combination of the orthogonal functions $\Psi_{\eta,(t_\eta)}$ and the individual products $\Psi_{\eta,(t_\eta)}\Psi_{\eta,(v_\eta)}$ give nonzero values only when $t=v$, when the above equation gives $\|\Psi_{\eta,(t_\eta)}\|_d^2$, which is the same as the one calculated in continuous space.

With the exception of a very few lattices, Gaussian-like quadratures do not give a Bravais discrete set $\boldsymbol{\mathcal{C}}_{oi}$. Nevertheless, if any regular set $\{\boldsymbol{e}_i\}$, giving a Bravais lattice, is chosen, the quadrature problem can be considered as to find the weights W_i and a scaling factor a such that $\boldsymbol{\mathcal{C}}_{o,i}=a\boldsymbol{e}_i$, satisfying Eq. (39). Considering that the poles $\boldsymbol{e}_i$ are previously known, this quadrature method was denoted as *quadrature with prescribed abcissas*.

In this manner, when the order of approximation N of the Hermite polynomial expansion to the MB equilibrium distribution is chosen, a set $\Psi_{\theta,(r_\theta)}$, $\theta=0,\ldots,N$, is established, and the infinite and enumerable basis of the Hilbert space $\mathcal{H}:c^D\to R$, which generates the solutions of the continuous Boltzmann equation, is replaced by a *finite* set of Hermite polynomial tensors, restricting the solutions to Nth-degree polynomials in the velocity $\boldsymbol{c}$. The quadrature problem is now to select a regular lattice $\{\boldsymbol{e}_i\}$ in such a manner that functions $\Psi_{\theta,(r_\theta)}$ preserve the orthogonality with respect to the inner product in the discrete space, and this can be accomplished by assuring that the norm of *each one* of these functions $\Psi_{\theta,(r_\theta)}$ is retrieved, *exactly*, in the discrete space. The number b of the required lattice vectors is dependent on the order N of the polynomial approximation, $b=b(N)$. In addition, we have shown that when the quadrature problem is solved, the 2θ-rank tensors given by Eq. (42) are isotropic in the discrete space for $\theta=1,\ldots,N$.

IV. TWO-DIMENSIONAL SQUARE LATTICES

We restrict our attention to two-dimensional square lattices, although the above presented quadrature procedure is general and may be used for deriving other two- or three-dimensional lattices.

When the equilibrium distribution is an Nth-order polynomial approximation to the MB distribution, quadrature will be exact for all moments of order $p\leqslant N$, if the weights W_iW are chosen so as to satisfy Eq. (39) for all the functions,

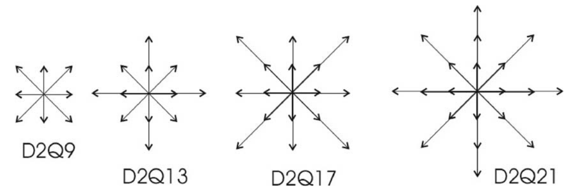

FIG. 2. Two-dimensional square lattices.

$$\Psi = \left\{1, 2C_{ox}, 2C_{oy}, 2\left(C_{ox}^2 - \frac{1}{2}\right), 2\left(C_{oy}^2 - \frac{1}{2}\right), 2C_{ox}C_{oy}, \ldots\right\}. \qquad (43)$$

Each one of these functions gives a quadrature equation. Some equations will be linearly dependent in accordance with the lattice symmetry.

In two dimensions, square lattices such as the D2Q9, D2Q13, and other DQ-like lattices have four discrete velocities at each energy level C_o. Figure 2 summarizes some square lattices that are being used in lattice Boltzmann simulation: each set of four discrete velocities is superposed to the previous lattice vectors set when adding a single energy level, following the sequence $(0,1,\sqrt{2},2,2\sqrt{2},3,3\sqrt{2},\ldots)$.

When $N=2$, there will be four linearly independent equations for four unknowns related to the scaling factor a, and the D2Q9 weights W_0, W_1, W_2. This set has a unique solution leading to the widely known values $W_0=16/36$, $W_1=4/36$, $W_2=1/36$, and $a=\sqrt{3/2}$. This is shown in Appendix B.

In this manner, a *second-order approximation* to the full MB distribution is the equilibrium distribution in the D2Q9 lattice, and this distribution may be written as a linear combination of the first *six* Hermite orthogonal polynomials Ψ_0, $\Psi_{1,x}$, $\Psi_{1,y}$, $\Psi_{2,xx}$, $\Psi_{2,yy}$, and $\Psi_{2,xy}$. The addition of further restrictions, related to the norm preservation of the third-order Hermite polynomials $\Psi_{3,xxy}$, $\Psi_{3,yyx}$, gives a system of equations with the same solution, but additional restrictions related to $\Psi_{3,xxx}$ or $\Psi_{3,yyy}$ gives a system *without solution*. Further, a ninth polynomial tensor that fits to the D2Q9 lattice can be found by considering a Gram-Schmidt orthogonalization of the function C_o^4, using the previous Hermite polynomials and the inner product Eq. (35). Nevertheless, the addition of these third- and fourth-order functions to the second-order polynomial expansion of the discrete equilibrium distribution f_i^{eq} does not appear to be helpful, since it does not change the order of approximation of f_i^{eq} and will not be considered in this paper.

The dimensionless local velocity $\boldsymbol{\mathcal{U}}_0=\boldsymbol{u}/(2kT_0/m)^{1/2}$ can be scaled to enable us to work with unitary lattice units. In this manner, the spatial and the time scales, h and δ, respectively, can be chosen so as to satisfy

$$\frac{h}{\delta} = \left(\frac{2kT_0}{m}\right)^{1/2}, \qquad (44)$$

and, since

$$\boldsymbol{\mathcal{U}}_0 = \sum_i f_i \boldsymbol{\mathcal{C}}_{oi} = a \sum_i f_i \boldsymbol{e}_i, \tag{45}$$

where $\boldsymbol{e}_i$ are the usual lattice vectors in 2D lattices, a new local velocity can be defined as

$$\boldsymbol{u}^* = \frac{\boldsymbol{\mathcal{U}}_0}{a} = \sum_i f_i \boldsymbol{e}_i. \tag{46}$$

The equilibrium distribution for the D2Q9 lattice is then

$$f_{i,2}^{\mathrm{eq}} = W_i n \left(1 + 2a^2 u_\alpha^* e_{i,\alpha} + 2a^2 u_\alpha^* u_\beta^* \left(a^2 e_{i,\alpha} e_{i,\beta} - \frac{1}{2}\delta_{\alpha\beta} \right) + \Theta(a^2 e_i^2 - 1) \right), \tag{47}$$

with third-order errors $O(\Theta u^*, u^{*3})$.

The effect of temperature on the equilibrium distribution can be clearly seen from Eq. (47). In higher temperature sites, the amount of rest particles is reduced and redistributed to higher energy levels, trying to mimic the temperature dependence of the continuous MB distribution. This effect is highly desirable in thermal LBE simulation. An equilibrium distribution similar to Eq. (47) is given as Eq. (18) of Shan and He [20].

When the macroscopic velocity $\boldsymbol{\mathcal{U}}_0$ is replaced by $\boldsymbol{u}^*$, the moments $a_{\theta,(r_\theta)}^{\mathrm{eq}}$ in Eqs. (25)–(29) are then

$$a_0^{\mathrm{eq}} = n, \tag{48}$$

$$a_{1,\alpha}^{\mathrm{eq}} = nau_\alpha^*, \tag{49}$$

$$a_{2,\alpha\beta}^{\mathrm{eq}} = na^2 u_\alpha^* u_\beta^* + \frac{1}{2} n\Theta\, \delta_{\alpha\beta}, \tag{50}$$

$$a_{3,\alpha\beta\gamma}^{\mathrm{eq}} = na^3 u_\alpha^* u_\beta^* u_\gamma^* + \frac{3}{2} n\Theta a u_\gamma^* \delta_{\alpha\beta}, \tag{51}$$

$$a_{4,\alpha\beta\gamma\delta}^{\mathrm{eq}} = na^4 u_\alpha^* u_\beta^* u_\gamma^* u_\delta^* + 3n\Theta a^2 u_\alpha^* u_\beta^* \delta_{\gamma\delta} + \frac{3}{4} n\Theta^2 \delta_{\alpha\beta}\delta_{\gamma\delta}. \tag{52}$$

In the same manner, the velocity functions $\Psi_{\theta,(r_\theta)}$ $(\boldsymbol{\mathcal{C}}_{o,i})$, Eqs. (12)–(16), can be rewritten in terms of the lattice vectors $\boldsymbol{e}_i$,

$$\Psi_0 = 1, \tag{53}$$

$$\Psi_{1,\alpha} = 2ae_{i\alpha}, \tag{54}$$

$$\Psi_{2,\alpha\beta} = 2\left(a^2 e_{i\alpha} e_{i\beta} - \frac{1}{2}\delta_{\alpha\beta} \right), \tag{55}$$

$$\Psi_{3,\alpha\beta\gamma} = \frac{4}{3}\left[a^3 e_{i\alpha} e_{i\beta} e_{i\gamma} - \frac{a}{2}(e_{i\alpha}\delta_{\beta\gamma} + e_{i\beta}\delta_{\alpha\gamma} + e_{i\gamma}\delta_{\alpha\beta}) \right], \tag{56}$$

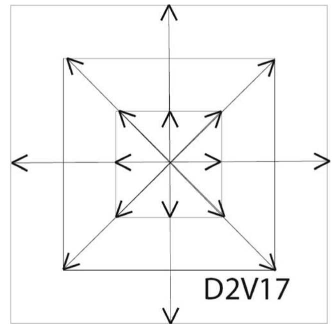

FIG. 3. The D2V17 lattice.

$$\Psi_{4,\alpha\beta\gamma\delta} = \frac{2}{3}\left[a^4 e_{i\alpha} e_{i\beta} e_{i\gamma} e_{i\delta} - \frac{a^2}{2}(e_{i\alpha} e_{i\beta}\delta_{\gamma\delta} + e_{i\alpha} e_{i\gamma}\delta_{\beta\delta} + e_{i\alpha} e_{i\delta}\delta_{\beta\gamma} + e_{i\beta} e_{i\gamma}\delta_{\alpha\delta} + e_{i\beta} e_{i\delta}\delta_{\alpha\gamma} + e_{i\gamma} e_{i\delta}\delta_{\alpha\beta}) + \frac{1}{4}\Delta_{\alpha\beta\gamma\delta} \right]. \tag{57}$$

The D2Q13 and the next lattices are also able to run second-order models. In these cases, the number of unknowns is greater than the number of disposable equations, and several solutions will be available, satisfying the quadrature problem.

Nevertheless, contrary to the results of McNamara and Alder [10] and to the results that would be expected with fitting methods (see Sec. IV), this lattice is *not able* to run *full* third-order models. Indeed, when $N=3$, it is impossible to find real positive values for a, W_0, W_1, W_2, W_3 satisfying all the norm restrictions, Eq. (39), related to $\Psi_{3,\alpha\beta\gamma}$. This result is the same for the D2Q17 lattice.

Considering the D2Q21 lattice as a next candidate for third-order models, there will be, in this case, seven unknowns a, W_0, W_1, W_2, W_3, W_4, W_5 for six norm restrictions, after eliminating identical equations. Letting a be a free variable, the system gives a solution with real positive roots when a is inside the interval $0.659836 \leqslant a \leqslant 1.16208$.

The values $a=0.659836$ and $a=1.16208$ (in fact, $a=1/12\sqrt{5}\sqrt{\sqrt{193}+25}$) are roots of the polynomials $W_0(a)$ and $W_3(a)$, respectively. In this manner, when the value $a=1.16208$ is chosen, $W_3=0$ and the lattice loses an energy level, giving a modification of the D2Q17 lattice, which has been named D2V17, shown in Fig. 3. The weights, with six significant digits, are $W_0=0.402005$, $W_1=0.116155$, $W_2=0.0330064$, $W_3=0$, $W_4=0.0000790786$, and $W_5=0.000258415$.

This modified square lattice is less expensive considering computer requirements and has the same properties when compared with the D2Q21 lattice, i.e., it retrieves, exactly, all the equilibrium moments up to the third order and gives isotropic tensors up to the sixth rank. Therefore, the present method can also be considered as a tool for investigating the structure of minimal velocity sets giving regular lattices. The D2V17 equilibrium distribution can be written as

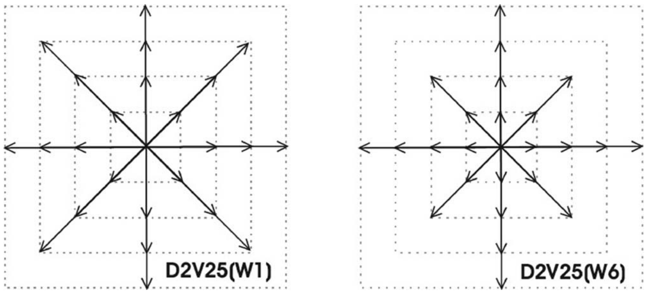

FIG. 4. The D2V25 lattices.

$$
\begin{aligned}
f^{\text{eq}}_{i,3} &= f^{\text{eq}}_{i,2} + W_i a^{\text{eq}}_{3,\alpha\beta\gamma}\Psi_{3,\alpha\beta\gamma}(i) \\
&= W_i n\Bigg[1 + 2a^2 u^*_\alpha e_{i,\alpha} + 2(a^2 u^*_\alpha u^*_\beta)\left(a^2 e_{i,\alpha}e_{i,\beta} - \frac{1}{2}\delta_{\alpha\beta}\right) \\
&\quad + \Theta(a^2 e_i^2 - 1) + \frac{4}{3}a^3 u^*_\alpha u^*_\beta u^*_\gamma\Bigg[a^3 e_{i,\alpha}e_{i,\beta}e_{i,\gamma} \\
&\quad - \frac{a}{2}(e_{i,\alpha}\delta_{\beta\gamma} + e_{i,\beta}\delta_{\alpha\gamma} + e_{i,\gamma}\delta_{\alpha\beta})\Bigg] \\
&\quad + 2\Theta a^2(a^2 e_i^2 - 2)u^*_\gamma e_{i,\gamma}\Bigg]
\end{aligned}
\tag{58}
$$

with fourth-order errors $O(\Theta u^{*2}, u^{*4})$.

In addition to the equilibrium moments up to third order, thermohydrodynamics requires the fourth-order equilibrium moments $\langle C_0^2 C_{0,x}^2\rangle^{\text{eq}}$, $\langle C_0^2 C_{0,y}^2\rangle^{\text{eq}}$, and $\langle C_0^2 C_{0,x}C_{0,y}\rangle^{\text{eq}}$ to be retrieved [10]. Since these functions are not orthogonal in the continuous velocity space, a Gram-Schmidt orthogonalization procedure was used to find orthogonal polynomials from this set by using the previous Hermite polynomials and the inner product Eq. (35).

The result was

$$\Psi_{4,1} = C_o^2 C_{o,x}^2 - \frac{7}{2}C_{o,x}^2 - \frac{1}{2}C_{o,y}^2 + 1, \tag{59}$$

$$\Psi_{4,2} = \frac{1}{7}[C_o^2(7C_{o,y}^2 - C_{o,x}^2) - 24C_{o,y}^2 + 6], \tag{60}$$

$$\Psi_{4,3} = C_{o,x}C_{o,y}(C_o^2 - 3). \tag{61}$$

When we require the norm preservation of the functions $\Psi_{4,1}$, $\Psi_{4,2}$, and $\Psi_{4,3}$, this gives a system of eight independent equations for nine unknowns. In this case, a is again a free parameter and the solution gave real positive weights for $0.590193 \leqslant a \leqslant 0.760569$.

Further, when a is, respectively, taken as 0.590193 or 0.760569, the weights W_1 or W_6 are null, giving two D2V25 lattices that retrieve the correct thermohydrodynamics equations. These lattices are shown in Fig. 4. For the first lattice, called D2V25(W1), $a=0.590193$ and the calculated weights are $W_0=0.235184$, $W_1=0$, $W=0.101817$, $W_3=5.92134\times 10^{-2}$, $W_4=2.00409\times 10^{-2}$, $W_5=6.79523\times 10^{-3}$, $W_6=1.14376\times 10^{-3}$, and $W_7=2.19788\times 10^{-3}$. Lattice D2V25(W6) has $a=0.760569$ and $W_0=0.239059$, $W_1=0.063158$, $W_2=8.75957\times 10^{-2}$, $W_3=3.11800\times 10^{-2}$, $W_4=6.19896\times 10^{-3}$, $W_5=2.02013\times 10^{-3}$, $W_6=0$, and $W_7=8.38224\times 10^{-5}$.

Therefore, thermohydrodynamic equations are correctly retrieved with the LBE based on these lattices, but isotropy of eighth-rank tensors cannot be assured. The equilibrium distribution for this lattice can be written as

$$f^{\text{eq}}_{i,\text{th}} = f^{\text{eq}}_{i,3} + W_i[a^{\text{eq}}_{4,1}\Psi_{4,1}(i) + a^{\text{eq}}_{4,2}\Psi_{4,2}(i) + a^{\text{eq}}_{4,3}\Psi_{4,3}(i)], \tag{62}$$

with, nevertheless, fourth-order errors $O(\Theta u^{*2}, u^{*4}, \Theta^2)$ with respect to the full MB distribution. Parameters $a^{\text{eq}}_{4,\theta}$ can be found by using the orthogonality properties of $\Psi_{4,\theta}$ ($\mathcal{C}_0$) in the continuous space, giving,

$$a^{\text{eq}}_{4,1} = \frac{2}{7}[2a^4 u_x^{*2}u^{*2} + \Theta a^2(6u_x^{*2} + u^{*2}) + 2\Theta^2], \tag{63}$$

$$a^{\text{eq}}_{4,2} = \frac{1}{12}(7a^4 u_y^{*4} - a^4 u_x^{*4} + 6a^4 u_x^{*2}u_y^{*2} + 24a^2 u_y^{*2}\Theta + 6\Theta^2), \tag{64}$$

$$a^{\text{eq}}_{4,3} = \frac{4}{3}a^2 u_x^* u_y^*(3\Theta + a^2 u^{*2}). \tag{65}$$

For the full fourth-order model, the norm preservation of a full set of Hermite orthogonal polynomials until the fourth order is required, giving a set of nine norm restrictions. This system will only be closed for a lattice with eight energy levels. The D2Q29 lattice, with eight weights $W_0, \ldots, W_7$, is a natural candidate to be the *minimal* square lattice to run fourth-order models in the square lattice hierarchy. For this lattice, there are nine linearly independent equations. This closed set of nine independent equations has, nevertheless, no solution.

This result was the same for the next D2Q33 lattice, when a is allowed to be a free parameter.

Since each function $\Psi_{\theta,(r_\theta)}$ is a linear combination of the monomials $\varphi=\{1, C_{ox}, C_{oy}, C_{ox}^2, C_{oy}^2, C_{ox}C_{oy}, \ldots\}$, the norm restrictions, Eq. (39), can be indifferently used on the set Ψ of orthogonal functions or on set φ of monomials. The last choice is, in the present case, preferable for identifying a symmetry deficiency in the DQ-series hierarchy of square lattices (Fig. 2). Indeed, consider the fourth-order functions $\varphi_{4,1}=C_{oy}^2 C_{ox}^2$ and $\varphi_{4,2}=C_{ox}^3 C_{oy}$. These functions have different norms in the continuous space, respectively, $3/4$ and $\sqrt{15/16}$. Nevertheless, since $\varphi_{4,1}=(C_{oy}C_{ox})^2$ and $\varphi_{4,2}=(C_{ox}C_{oy})C_{ox}^2$, the only contributions for their norms in the discrete space came from the diagonal vectors and are the same because along these directions $|C_{o,iy}|=|C_{o,ix}|$.

This is an important result, since it means that the Q-series of square lattices are unable to run full fourth-order LBE models.

In this way, we have tried another building structure for the lattices, filling completely the available Cartesian space around each site following the sequence $|e_i|=0, 1, \sqrt{2}, 2, \sqrt{5}, 2\sqrt{2}, 3, \sqrt{10}$ with sequentially increasing values for $|e_i|$.

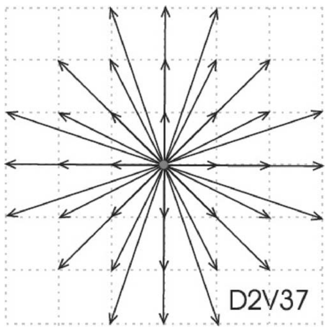

FIG. 5. The D2V37 lattice.

Figure 5 shows a D2V37 lattice, constructed in such a manner, with 37 velocity vectors but eight weights W_i. Solution of the nine norm equations is unique and gives, when six significant digits are considered, $a=0.846393$, $W_0=0.233151$, $W_1=0.107306$, $W_2=0.0576679$, $W_3=0.0142082$, $W_4=0.00535305$, $W_5=0.00101194$, $W_6=0.000245301$, and $W_7=0.000283414$. This lattice came from the solution of a closed system with nine linearly independent norm restriction for nine unknowns.

Since, in the D2V37 lattice, all the fourth-order Hermite polynomial tensors belong to the orthogonal basis of this lattice, the equilibrium distribution can be written as

$$\begin{aligned} f_{i,4}^{\text{eq}} &= f_{i,3}^{\text{eq}} + W_i a_{4,\alpha\beta\gamma\delta}^{\text{eq}} \Psi_{4,\alpha\beta\gamma\delta}(i) \\ &= W_i n \Bigg\{ 1 + 2a^2 u_\alpha^* e_{i,\alpha} + 2(a^2 u_\alpha^* u_\beta^*)\left(a^2 e_{i,\alpha} e_{i,\beta} - \frac{1}{2}\delta_{\alpha\beta}\right) \\ &\quad + \Theta(a^2 e_i^2 - 1) + \frac{4}{3} a^3 u_\alpha^* u_\beta^* u_\gamma^* \Bigg[a^3 e_{i,\alpha} e_{i,\beta} e_{i,\gamma} \\ &\quad - \frac{a}{2}(e_{i,\alpha}\delta_{\beta\gamma} + e_{i,\beta}\delta_{\alpha\gamma} + e_{i,\gamma}\delta_{\alpha\beta}) \Bigg] + 2\Theta a^2 (a^2 e_i^2 - 2) u_\gamma^* e_{i,\gamma} \\ &\quad + \frac{2}{3}\Bigg[\Bigg[a^8 (u_\alpha^* e_{i\alpha})^4 - 3a^6 u^{*2} (u_\alpha^* e_{i\alpha})^2 + \frac{3}{4} a^4 u^{*4} \Bigg] \\ &\quad + \Theta \Bigg[3a^6 (u_\alpha^* e_{i\alpha})^2 e_i^2 - \frac{3}{2} a^4 [D(u_\alpha^* e_{i\alpha})^2 + 4(u_\alpha^* e_{i\alpha})^2 \\ &\quad + u^{*2} e_i^2] + \frac{3}{4} a^2 u^{*2} (D+2) \Bigg] \\ &\quad + \frac{3}{4}\Theta^2 \Bigg[a^4 e_i^4 - \frac{1}{2} a^2 (D+2) e_i^2 + \frac{1}{4} D(D+2) \Bigg]\Bigg]\Bigg\}. \end{aligned} \tag{66}$$

The D2V37 lattice, with the above equilibrium distribution, can be considered as the *minimal* square lattice giving a fourth-order approximation to the continuous Boltzmann equation, wih errors $O(\Theta^2 u^*, u^{*5})$.

The weights W_i, in general, decrease with i and attain very small values when i is large. The smallness of W_i for large i is expected and is a consequence of (a) the restriction that was imposed on the lattice to be space filling, requiring the norm of each added lattice vector, $\boldsymbol{e}_i$ to be, frequently, an integer multiple of the norm of the lattice vectors forming the D2Q9 lattice unitary cell in square lattices, and (b) the required degree of approximation leading to polynomials with terms of $O(e_b^N)$.

V. DISCUSSION: A DISCRETIZATION APPROACH BASED ON A FINITE SET OF ORTHOGONAL FUNCTIONS IN THE DISCRETE SPACE

Consider a previously assigned velocity set $\ell=\{\boldsymbol{c}_0,\ldots,\boldsymbol{c}_b\}$ giving a regular lattice. Returning to Eq. (1),

$$\langle\varphi_\eta\rangle^{\text{eq}} = \int \frac{f^{\text{eq}}(\boldsymbol{c})}{n_d}\varphi_\eta(\boldsymbol{c})d\boldsymbol{c} = \sum_i \frac{f_i^{\text{eq}}}{n}\varphi_\eta(\boldsymbol{c}_i) \tag{67}$$

for $\eta=0,1,2,\ldots,b$, but now φ_η forms a set of $b+1$ linearly independent velocity monomials in a given lattice with $b+1$ degrees of freedom. Considering, e.g., the D2Q9 lattice, this set can be chosen as

$$\varphi = \{1, c_{ix}, c_{iy}, c_{ix}^2, c_{iy}^2, c_{ix}c_{iy}, c_{ix}^2 c_{iy}, c_{iy}^2 c_{ix}, c_i^4\}, \tag{68}$$

since, in this lattice, there are only two third-degree linearly independent monomials and a fourth-degree additional monomial is required.

The orthogonal functions $\Psi_{\theta,(r_\theta)}(\boldsymbol{c}_i)$ are now considered to be derived from the set φ_η. This can be accomplished by using an orthogonalization procedure, such as the Gram-Schmidt process, and is the basis of the LB moments method [13]. Since the particular forms of $\Psi_{\theta,(r_\theta)}(\boldsymbol{c}_i)$ are dependent on the lattice, on functions φ_η, and on the manner in which the Gram-Schmidt method is used, these functions will be noted as $\Psi^\ell_{\theta,(r_\theta)}(\boldsymbol{c}_i)$ to distinguish them from the above Hermite polynomial tensors.

In this case, an inner product must be defined in the discrete space generated by the functions $f:\{\boldsymbol{c}_0,\ldots,\boldsymbol{c}_b\}\to R$. Considering

$$(a * b)_d = \sum_i a_i b_i \tag{69}$$

to be such a product each element of the orthogonal basis can be written in terms of the monomials φ_η as

$$\Psi^\ell_{\theta,(r_\theta)} = \sum_{\eta=0}^{\theta} a^{\theta,\ell}_{\eta,(s_\eta)}\varphi_\eta, \tag{70}$$

where $a^{\theta,\ell}_{\eta,(s_\eta)}$ are real numbers, dependent on the assigned lattice. After multiplying Eq. (67) by $a^{\theta,\ell}_{\eta,(s_\eta)}$ for each η and adding the resulting equations, we obtain

$$\int \frac{f^{\text{eq}}(\boldsymbol{c})}{n_d}\Psi^\ell_{\theta,(r_\theta)}(\boldsymbol{c})d\boldsymbol{c} = \sum_i \frac{f_i^{\text{eq}}}{n}\Psi^\ell_{\theta,(r_\theta)}(\boldsymbol{c}_i). \tag{71}$$

Expanding f_i^{eq}/n in terms of functions $\Psi^\ell_{\theta,(r_\theta)}(\boldsymbol{c}_i)$,

$$\frac{f_i^{\text{eq}}}{n} = \sum_{\theta=0}^{b} a^{\text{eq},\ell}_{\theta,(r_\theta)}\Psi^\ell_{\theta,(r_\theta)}(\boldsymbol{c}_i). \tag{72}$$

Since $\Psi^\ell_{\theta,(r_\theta)}(\boldsymbol{c}_i)$ are orthogonal (in the discrete space), the following relationship follows directly from Eq. (71):

$$\int \frac{f^{\mathrm{eq}}(\boldsymbol{c})}{n_d} \Psi^{\ell}_{\theta,(r_\theta)}(\boldsymbol{c}) d\boldsymbol{c} = a^{\mathrm{eq},\ell}_{\theta,(r_\theta)} \lambda_\theta, \tag{73}$$

where

$$\lambda_\theta = \sum_i (\Psi^{\ell}_{\theta,(r_\theta)})^2, \tag{74}$$

resulting in

$$a^{\mathrm{eq},\ell}_{\theta,(r_\theta)} = \frac{\displaystyle\int \frac{f^{\mathrm{eq}}(\boldsymbol{c})}{n_d} \Psi^{\ell}_{\theta,(r_\theta)}(\boldsymbol{c}) d\boldsymbol{c}}{\displaystyle\sum_i (\Psi^{\ell}_{\theta,(r_\theta)})^2}. \tag{75}$$

The above equation gives the equilibrium moment $a^{\mathrm{eq},\ell}_{\theta,(r_\theta)}$ in terms of the MB distribution function for a given order θ of the function $\Psi^{\ell}_{\theta,(r_\theta)}$.

In this manner, Eq. (71) can be regarded as a *discretization equation* giving the unknowns f_i^{eq} in terms of the MB distribution function, requiring the moments $a^{\mathrm{eq},\ell}_{\theta,(r_\theta)}$ to be the projections of the full MB distribution, $f^{\mathrm{eq}}(\boldsymbol{c})$, on a (not orthogonal) basis $\Psi^{\ell}_{\theta,(r_\theta)}(\boldsymbol{c})$ of $\mathcal{H}_N$, Eq. (75).

The discrete velocities $\boldsymbol{c}_i$ can be related to the dimensionless lattice vectors $\mathbf{e}_i$ through

$$\boldsymbol{c}_i = \frac{h}{\delta} \boldsymbol{e}_i, \tag{76}$$

where h and δ are, respectively, the space and time scales.

The next step is now to find the polynomial approximation, $f_N^{\mathrm{eq}}(\boldsymbol{c})$, to the full MB equilibrium distribution that is generated by functions $\Psi^{\ell}_{\theta,(r_\theta)}(\boldsymbol{c})$ of $\mathcal{H}_N$ and see what is the relationship between $f_N^{\mathrm{eq}}(\boldsymbol{c}_i)$ and the above derived f_i^{eq}.

It is important to emphasize that although functions $\Psi^{\ell}_{\theta,(r_\theta)}$ are orthogonal in the subspace $\mathcal{H}_N$ of $\mathcal{H}$, generated by $\Psi^{\ell}_{\theta,(r_\theta)}$ with respect to the inner product, Eq. (69), these functions are, in general, *not orthogonal* in this subspace, with respect to the inner product of $\mathcal{H}$, Eq. (17). Thus, consider replacing $f^{\mathrm{eq}}(\boldsymbol{c})$ on the left-hand side of Eq. (73) by the projection $f_N^{\mathrm{eq}}(\boldsymbol{c})$ of the MB distribution on the subspace spanned by functions $\Psi^{\ell}_{\theta,(r_\theta)}(\boldsymbol{c})$.

Written in terms of $\Psi^{\ell}_{\eta,(s_\eta)}$, this projection will have a form analogous to Eq. (18),

$$f_N^{\mathrm{eq}} = n_d \frac{e^{-\mathcal{C}^2}}{\pi^{D/2}} \left(\frac{m}{2kT} \right)^{D/2} \sum_{\theta=0}^{N} a^{\mathrm{eq},\ell}_{\eta,(s_\eta)} \Psi^{\ell}_{\eta,(s_\eta)}(\boldsymbol{\mathcal{C}}). \tag{77}$$

Since functions $\Psi^{\ell}_{\eta,(s_\eta)}$ are not orthogonal with respect to Eq. (17), Eq. (73) gives

$$\sum_\eta a^{\mathrm{eq},\ell}_{\eta,(s_\eta)} \frac{1}{\pi^{D/2}} \int e^{-\mathcal{C}^2} \Psi^{\ell}_{\eta,(s_\eta)} \Psi^{\ell}_{\theta,(r_\theta)} d\boldsymbol{\mathcal{C}} = a^{\mathrm{eq},\ell}_{\theta,(r_\theta)} \lambda_\theta, \tag{78}$$

which is a closed system of equations for the unknows $a^{\mathrm{eq},\ell}_{\eta,(s_\eta)}$. When $a^{\mathrm{eq},\ell}_{\theta,(r_\theta)}$ on the right-hand side of the above equation is considered to be either given by Eq. (75) or to be unknown, this system can only be expected to have the same solution, Eq. (75), when functions $\Psi^{\ell}_{\eta,(s_\eta)}$ are orthogonal with respect to the inner product Eq. (17) and

$$\frac{1}{\pi^{D/2}} \int e^{-\mathcal{C}^2} \Psi^{\ell}_{\eta,(s_\eta)} \Psi^{\ell}_{\theta,(r_\theta)} d\boldsymbol{\mathcal{C}} = \sum_i \Psi^{\ell}_{\eta,(s_\eta)}(\boldsymbol{\mathcal{C}}_i) \Psi^{\ell}_{\theta,(r_\theta)}(\boldsymbol{\mathcal{C}}_i), \tag{79}$$

which is not generally true.

This means that, analogous to the previous approach discussed in the beginning of Sec. I, $f_N^{\mathrm{eq}}(\boldsymbol{c})$ has no identification with f_i^{eq} and does not converge to f_i^{eq} (or to a weighted f_i^{eq}) when $\boldsymbol{c}$ approaches the poles $\boldsymbol{c}_i$.

In this manner, although the above exposed discretization procedure leads to the correct macroscopic equilibrium moments and, as a consequence, to the correct hydrodynamic equations, the generated discrete equilibrium distribution loses any local identification with its continuous counterpart.

LBM is a kinetic method based on the solution of a discrete kinetic equation (and not on the solution of the hydrodynamic equations themselves), and the next question to be answered is, to what extent does this lack of identification affect the solution of a given hydrodynamic problem?

VI. CONCLUSION

The present paper deals with the discretization problem in generating the lattice Boltzmann equation from the continuous Boltzmann equation.

In the quadrature problem, lattices with temperature-dependent particle velocities were avoided by letting the particle velocity, c^2, be free from the temperature T in the exponential part e^{-C^2} of the MB distribution and writing the equilibrium distribution as a Taylor expansion in terms of the temperature deviation Θ.

It was shown that the LBE can be derived from the continuous Boltzmann equation when the orthogonality of the Hermite polynomial tensors in the continuous space is maintained. It was also shown that this can be assured when the norms of these tensors are preserved in discrete space, leading to increasingly accurate lattice Boltzmann models.

In this manner, the preservation of the functional structure of the Hilbert space, $\mathcal{H}_N$, when its inner product and induced norm are replaced by discrete sums, appears to be a fundamental rule for the velocity discretization problem when the discrete equilibrium distribution is required to give increasingly accurate approximations with respect to the continuous MB distribution. Although equilibrium moments are preserved, this rule is not, in general, satisfied by the lattices, which structure is derived from a finite polynomial expansion in the discrete space.

These restrictions lead to space-filling lattices with increased dimensionality when compared with presently known square lattices. In this manner, it was concluded that a 17-velocities lattice is required for third order and a 25-velocities lattice is needed for thermal model approximations, compared with, respectively, the D2Q13 and D2Q17 lattices, which are shown to retrieve the correct macroscopic equations related to these moments. In particular, considering thermal problems, the D2Q17 lattice, which equilibrium distributions f_i^{eq} are obtained with the method exposed in Sec.

TABLE I. Parity indexes of some leading Hermite polynomial tensors.

$\Psi_{\theta,(r_\theta)}$	m_x	m_y
Ψ_0	0	0
$\Psi_{1,x}$	1	0
$\Psi_{1,y}$	0	1
$\Psi_{2,xx}$	2	0
$\Psi_{2,yy}$	0	2
$\Psi_{2,xy}$	1	1
$\Psi_{3,xxx}$	3	0
$\Psi_{3,xyy}$	1	2
$\Psi_{3,yyy}$	0	3

IV, retrieves the thermohydrodynamic equations, but its equilibrium distribution and the derived lattice Boltzmann equation cannot be considered as reliable approximations to the MB distribution and the Boltzmann equation, respectively.

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APPENDIX A: ORTHOGONALITY OF THE HERMITE POLYNOMIAL TENSORS IN THE DISCRETE SPACE

Let $\Psi_{\theta,(r_\theta)}$ be a set of Hermite polynomial tensors, orthogonal with respect to the inner product Eq. (35). Consider a Bravais lattice, where to each velocity vector $\mathcal{C}_{0,i}$, $\mathcal{C}_{0,i} \neq 0$, corresponds a discrete velocity $\mathcal{C}_{0,-i}=-\mathcal{C}_{0,i}$.

Let $m_\alpha(\Psi_{\theta,(r_\theta)})$ be a parity index giving the number of times the index α appears in $\Psi_{\theta,(r_\theta)}$. Table I gives the parity indexes of some leading Hermite polynomial tensors in two dimensions.

Index $m_\alpha(\Psi_{\theta,(r_\theta)})$ gives the parity of $\Psi_{\theta,(r_\theta)}$ with respect to the α component of the particle velocity $\mathcal{C}_0$. In this manner, the Hermite polynomials $\Psi_{\theta,(r_\theta)}$ can be also written as a three-index function $\Psi_{\theta,m_{x\theta},m_{y\theta}}$. This last notation is more convenient for the present purpose.

When making the inner product in either its continuous, Eq. (35), and discrete, Eq. (36), forms,

$$(\Psi_{\theta,m_{x\theta},m_{y\theta}} * \Psi_{\eta,m_{x\eta},m_{y\eta}})_{c \text{ or } d'},$$

this product is trivially null whenever

$$m_x(\Psi_{\theta,m_{x\theta},m_{y\theta}}\Psi_{\eta,m_{x\eta},m_{y\eta}}) = m_{x\theta}+m_{x\eta}$$

or

$$m_y(\Psi_{\theta,m_{x\theta},m_{y\theta}}\Psi_{\eta,m_{x\eta},m_{y\eta}}) = m_{y\theta}+m_{y\eta}$$

are odd.

When both parity indexes $m_x(\Psi_{\theta,m_{x\theta},m_{y\theta}}\Psi_{\eta,m_{x\eta},m_{y\eta}})$ and $m_y(\Psi_{\theta,m_{x\theta},m_{y\theta}}\Psi_{\eta,m_{x\eta},m_{y\eta}})$ are even, the resulting polynomial is invariant under changes $C_{0x}\to -C_{0x}$ and $C_{0y}\to -C_{0y}$, therefore it has only quadratic forms in the monomials 1, C_{0x}, C_{0y}, C_{0x}^2, C_{0y}^2, $\mathcal{C}_{0x}\mathcal{C}_{0y},\ldots$. When both parity indexes $m_x(\Psi_{\theta,m_{x\theta},m_{y\theta}}\Psi_{\eta,m_{x\eta},m_{y\eta}})$ and $m_y(\Psi_{\theta,m_{x\theta},m_{y\theta}}\Psi_{\eta,m_{x\eta},m_{y\eta}})$ are even, the resulting polynomial is invariant under changes $C_{0x}\to -C_{0x}$ and $C_{0y}\to -C_{0y}$, therefore it has only quadratic forms in the monomials

$$C=\{C_{\theta,m_{x\theta},m_{y\theta}}=1, C_{0x}, C_{0y}, C_{0x}^2, C_{0y}^2, C_{0x}C_{0y}, \ldots\}$$

. The squared monomials can be written as linear combinations of $\Psi_{i,j,k}^2$. This comes from the consideration that each square $\Psi_{\theta,m_{x\theta},m_{y\theta}}^2$ depends on a leading term related to $C_{\theta,m_{x\theta},m_{y\theta}}^2$ and on lower-order degree monomials. In this manner, letting Ψ^2 and C^2 be vectors,

$$\Psi^2 = [\Psi_0^2, \Psi_{1,1,0}^2, \ldots, \Psi_{\theta,m_{x\theta},m_{y\theta}}^2]$$

and

$$C^2 = [C_0^2, C_{1,1,0}^2, \ldots, C_{\theta,m_{x\theta},m_{y\theta}}^2],$$

respectively, the linear system of equations

$$\Psi^2 = AC^2 \tag{A1}$$

can be easily inverted since A is a triangular matrix, with non-null terms in the diagonal. Consequently, the products will be

$$\Psi_{\theta,m_{x\theta},m_{y\theta}}\Psi_{\eta,m_{x\eta},m_{y\eta}} = \sum_{i=0}^{(\theta+\eta)/2}\sum_{j=0}^{i} a_{i,j,i-j}\Psi_{i,j,i-j}^2, \tag{A2}$$

where the parameters $a_{i,j,i-j}$ are constants.

As a consequence, when $(\Psi_{\theta,m_{x\theta},m_{y\theta}} * \Psi_{\eta,m_{x\eta},m_{y\eta}})_d$ is not trivially null, i.e., when $m_x(\Psi_{\theta,m_{x\theta},m_{y\theta}}\Psi_{\eta,m_{x\eta},m_{y\eta}})$ and $m_y(\Psi_{\theta,m_{x\theta},m_{y\theta}}\Psi_{\eta,m_{x\eta},m_{y\eta}})$ are even, this inner product will be given by

$$\begin{aligned}(\Psi_{\theta,m_{x\theta},m_{y\theta}} * \Psi_{\eta,m_{x\eta},m_{y\eta}})_d &= \sum_{i=0}^{(\theta+\eta)/2}\sum_{j=0}^{i} a_{i,j,i-j}\|\Psi_{i,j,i-j}\|_d^2 = \sum_{i=0}^{(\theta+\eta)/2}\sum_{j=0}^{i} a_{i,j,i-j}\|\Psi_{i,j,i-j}\|_c^2 \\ &= (\Psi_{\theta,m_{x\theta},m_{y\theta}} * \Psi_{\eta,m_{x\eta},m_{y\eta}})_c\end{aligned} \tag{A3}$$

because (i) the norms of functions Ψ_θ are preserved and (ii) Eq. (A2) is true in both continuous and discrete space.

In this manner, since functions Ψ_θ are orthogonal in continuous space, they will also be orthogonal in discrete space with respect to the inner product, Eq. (36).

This result can be easily generalized for three-dimensional lattices.

APPENDIX B

Considering the D2Q9 lattice, the norm and orthogonality restrictions give for the functions

$$\{\Psi_0, \Psi_{1,x}, \Psi_{1,y}, \Psi_{2,xx}, \Psi_{2,yy}, \Psi_{2,xy}\} \tag{B1}$$

the following system of equations:

$$\frac{1}{\pi}\left[\int_{-\infty}^{\infty} e^{-C_{0y}^2}\left(\int_{-\infty}^{\infty} e^{-C_{0x}^2} 1 dC_{0x}\right) dC_{0y}\right] = 1 = W_0 + 4W_1 + 4W_2,$$

$$\frac{1}{\pi}\left[\int_{-\infty}^{\infty} e^{-C_{0y}^2}\left(\int_{-\infty}^{\infty} e^{-C_{0x}^2}(2C_{0x})^2 dC_{0x}\right) dC_{0y}\right] = 2 = 8a^2W_1 + 16a^2W_2,$$

$$\frac{1}{\pi}\left(\int_{-\infty}^{\infty} e^{-C_{0y}^2}\left\{\int_{-\infty}^{\infty} e^{-C_{0x}^2}\left[2\left(C_{0x}^2-\frac{1}{2}\right)\right]^2 dC_{0x}\right\} dC_{0y}\right) = 2 = W_0 + 4W_2(2a^2-1)^2 + W_1[2(2a^2-1)^2+2],$$

$$\frac{1}{\pi}\left[\int_{-\infty}^{\infty} e^{-C_{0y}^2}\left(\int_{-\infty}^{\infty} e^{-C_{0x}^2}(2C_{0x}C_{0y})^2 dC_{0x}\right) dC_{0y}\right] = 1 = 16a^4W_2,$$

$$\frac{1}{\pi}\left\{\int_{-\infty}^{\infty} e^{-C_{0y}^2}\left[\int_{-\infty}^{\infty} e^{-C_{0x}^2} 1 \times 2\left(C_{0x}^2-\frac{1}{2}\right) dC_{0x}\right] dC_{0y}\right\} = 0 = W_1(4a^2-4) - W_0 + W_2(8a^2-4),$$

$$\frac{1}{\pi}\left\{\int_{-\infty}^{\infty} e^{-C_{0y}^2}\left[\int_{-\infty}^{\infty} e^{-C_{0x}^2} 2\left(C_{0x}^2-\frac{1}{2}\right) \times 2\left(C_{0y}^2-\frac{1}{2}\right) dC_{0x}\right] dC_{0y}\right\} = 0 = W_0 + W_1(4-8a^2) + 4W_2(2a^2-1)^2,$$

where identical equations and the inner products giving odd velocity functions were previously excluded.

There are only four independent equations. The solution of the above system gives the classically known values $a=\sqrt{3/2}$, $W_0=16/36$, $W_1=4/36$, and $W_2=1/36$, which are also the solutions when only the first four equations, related to the norm restrictions, are considered. In this manner, the two linearly independent orthogonality conditions are satisfied by the solution of the norm equations. This outcome was the same for all the lattice that have been analyzed in this work, and Appendix A shows that this result is, in fact, a consequence of general properties of Hermite polynomials and of the Bravais lattices structure.

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