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General solution of lattices for Cartesian lattice Bhatanagar-Gross-Krook models

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We give the general solutions of lattices, i.e., velocity sets and weights, for the lattice Bhatanagar-Gross-Krook (LBGK) models on two- and three-dimensional Cartesian grids. The solutions define the necessary and sufficient conditions so that the resulting LBGK model can accurately capture the dynamics of the moments retained in the distribution function. In the parameter space of the weights, the general solutions form low-dimensional linear spaces from which minimal velocity sets are identified for the degrees of precision that are most relevant to the construction of high-order LBGK models. All well-known LBGK lattices are found to be special cases of the given general solutions.

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I. INTRODUCTION

As the statistical mechanical foundation of thermohydrodynamic equations, the Boltzmann kinetic equation describes the physics of fluids at a more fundamental level and applies in a wider domain. Despite the tremendous growth of computing power in recent years, direct simulation of the kinetic equation remains too cost prohibitive for most engineering applications. Discrete-velocity kinetic models [1] have been sought after where the entire three-dimensional (3D) velocity space is approximated by a small number of discrete velocities. The lattice Boltzmann (LB) method [2,3], although historically derived from the lattice gas cellular automaton, has also been shown to be a special velocity-space discretization of the Boltzmann-BGK equation [4]. For this class of models to be successful, the macroscopic behavior of the kinetic equation must be preserved by the discretization of the velocity space. It has been shown that the macroscopic behavior of the lattice Bhatanagar-Gross-Krook (LBGK) equation well approximates that of the continuum Boltzmann-BGK equation provided that the discrete velocities form a Gauss-Hermite quadrature in the velocity space with a sufficient degree of precision [5]. Once space and time are also discretized, the discrete velocities effectively define the *lattice* of the LBGK model. In the discussion hereinafter, we shall use *lattice* and *discrete velocities* indistinguishably.

The standard LBGK models [6,7] employ lattices that are only accurate for restoring the Navier-Stokes momentum equation at the near-incompressible limit. Recently more accurate lattices are found to be critical in recovering higher-order hydrodynamics such as the energy equation [8,9], the Galilean invariance of the transport coefficients [10], and the behaviors beyond the Navier-Stokes order [11–14]. In one dimension (1D), the Gauss-Hermite quadrature are established by the fundamental theorem of Gauss quadrature. However, no general solutions are known in higher dimensions except for the "product" formulas which are constructed as the tensor product of 1D formulas and often use much larger velocity sets than necessary. Using various techniques, many quadratures with smaller velocity sets were obtained case by case [15], For the low dimension and degree of precision relevant to the construction of LBGK models, those specially obtained quadratures are believed to be minimal. However, the special quadratures usually have abscissas not coincide with regular lattices, making them less desirable choices in LBGK models for both accuracy and efficiency reasons.

It was pointed out previously [5,8,16] that quadratures with predefined Cartesian abscissas can be obtained exhaustively by solving the orthogonality relations. Based on the entropy construction [17] and factorization of symmetry, Chikatamarla and Karlin suggested another approach [18–20] in which the higher-dimensional product velocity sets are pruned to smaller sets while preserving the essential hydrodynamic moments. More recently, it was also noticed that the same condition pertaining to discrete-velocity sets can be obtained using symmetry arguments [21]. Although a number of high-order lattices are obtained using the different approaches and found to be very effective in extending the application domain of the LB method, the comprehensiveness and minimality of those lattices have not been established in general, neither are the connections among the different approaches identified.

Aiming at these remaining issues, in this paper, we give the general solutions of Cartesian lattices using the previously defined quadrature approach [5]. We first outline the relation between the degree of precision of a quadrature and the order of accuracy of the corresponding LBGK model, defined as the order of the highest moments of which the dynamics are accurately captured. Quadratures with Cartesian abscissas are then solved from the necessary and sufficient conditions for the leading moments of the distribution function to be exactly representable by the discrete velocities. The general solutions of lattices are found to form linear subspaces in the parameter space of the quadrature weights. The minimal velocity sets required for each order of accuracy are found by keeping the least populous symmetry groups. When positivity of the quadrature weights are required for the purpose of constructing numerically stable LBGK models, the problem of finding the minimum LBGK lattice is reduced to a problem of linear programming. We also compare some well-known LBGK lattices with the general solutions obtained.

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II. QUADRATURES AND HYDRODYNAMICS

Our discussion starts with the continuum Boltzmann-BGK equation. Following the previous nondimensionalization convention [5], it can be written as

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla f = -\frac{1}{\tau}[f - f^{(0)}], \tag{1}$$

where $f = f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ is the single-particle distribution function in the phase space $(\boldsymbol{x}, \boldsymbol{\xi}, t)$; $\boldsymbol{x}$, $\boldsymbol{\xi}$, and t are the spatial coordinate, microscopic velocity and time respectively, τ the relaxation time, and $f^{(eq)}$ the Maxwell-Boltzmann distribution,

$$f^{(0)} = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left[-\frac{|\boldsymbol{u} - \boldsymbol{\xi}|^2}{2\theta}\right]. \tag{2}$$

where ρ, $\boldsymbol{u}$, and θ are the nondimensional hydrodynamic variables of density, velocity and temperature.

Choosing the Hermite polynomials [22] as the expansion basis, solving Eqs. (1) and (2) calls for projecting them into the Hilbert space spanned by the leading Hermite polynomials [5], e.g., the single-particle distribution f is approximated by a finite Hermite series,

$$f \cong f^N \equiv \omega(\boldsymbol{\xi}) \sum_{n=0}^{N} \frac{1}{n!} \boldsymbol{a}^{(n)}(\boldsymbol{x}, t) \mathcal{H}^{(n)}(\boldsymbol{\xi}), \tag{3}$$

where $\mathcal{H}^{(n)}(\boldsymbol{\xi})$ is the nth Hermite polynomial, $\boldsymbol{a}^{(n)}$ the expansion coefficient, and $\omega(\boldsymbol{\xi})$ the weight function:

$$\omega(\boldsymbol{\xi}) = \frac{1}{(2\pi)^{D/2}} e^{-\xi^2/2}. \tag{4}$$

Essentially two facts allow Eq. (1) to be discretized in velocity space to give the LBGK equations. First, when Chapman-Enskog calculation is carried out on Eq. (1), only the leading-order moments of f appear in the hydrodynamic equations. The order of the highest relevant moment is determined by the physics of interest and the order of hydrodynamic approximation [5]. For instance, the momentum flux and heat flux are respectively the second and third moments of the distribution function. At the first (Navier-Stokes) hydrodynamic approximation, moments up to one order higher, e.g., third and fourth moments, are needed so that the transport of momentum and heat in the discrete-velocity kinetic equation is the same as that in the continuum version. Second, for distributions of the form of Eq. (3), the moments are given by the discrete values of the distribution function via the Gauss-Hermite quadratures. Let $\{(w_i, \boldsymbol{\xi}_i): i = 1, \ldots, d\}$ be the pairs of weight and abscissa of a quadrature such that for any polynomial $\boldsymbol{p}(\boldsymbol{\xi})$ of an order not exceeding Q, we have

$$\int \omega(\boldsymbol{\xi}) \boldsymbol{p}(\boldsymbol{\xi}) d\boldsymbol{\xi} = \sum_{i=1}^{d} w_i \boldsymbol{p}(\boldsymbol{\xi}_i), \tag{5}$$

where Q is known as the *degree of precision* of the quadrature. Let M be the order of the highest relevant moments and $\boldsymbol{\xi}^M$ the tensor product of $\boldsymbol{\xi}$ by itself for M times. Obviously the expansion must retain all relevant moments, i.e., $N \geq M$. Since $f^N(\boldsymbol{\xi})\boldsymbol{\xi}^M / \omega(\boldsymbol{\xi})$ is a polynomial of an order not exceeding $M+N$, as long as $M+N \leq Q$, we have

$$\int f^N \boldsymbol{\xi}^M d\boldsymbol{\xi} = \sum_{i=1}^{d} \frac{w_i f^N(\boldsymbol{\xi}_i) \boldsymbol{\xi}_i^M}{\omega(\boldsymbol{\xi}_i)}. \tag{6}$$

The conditions for the discrete-velocity kinetic equation to recover the correct hydrodynamics are therefore [10]

$$N \geq M \quad \text{and} \quad M + N \leq Q, \tag{7}$$

which is to be compared with the similar condition given by Chikatamarlar and Karlin [19]. In standard LBGK models, $Q=5$ and $M=2$ out of the minimum requirement of recovering the Navier-Stokes momentum equation. The truncation order is either two or three with the former being the standard in almost all implementations. With a higher-order lattice, the truncation order is allowed to vary more independent of the quadrature order.

We notice that since all polynomials of orders not exceeding N form a linear space, say $\mathcal{P}^N$. Equation (5) is true for any $\boldsymbol{p} \in \mathcal{P}^N$ if and only if it is true for a set of basis of $\mathcal{P}^N$. Since the Hermite polynomials form a basis of $\mathcal{P}^N$, letting $\boldsymbol{p} = \mathcal{H}^{(n)}$ and carrying out the integrals on the left-hand side of Eq. (5), the weights of a degree-N quadrature, w_i, can be solved from the following equations:

$$\sum_{i=1}^{d} w_i \mathcal{H}^{(n)}(\boldsymbol{\xi}_i) = \begin{cases} 1 & n = 0 \\ 0 & n \neq 0 \end{cases}, \quad \forall\, n \leq Q. \tag{8}$$

Equation (8) is the necessary and sufficient condition for any set of abscissas and their associated weights to form a Hermite quadrature whether the abscissas fall on a Cartesian grid or not. For any predefined abscissas, including the particularly interesting class that form Bravias lattices, the corresponding weights can be explicitly solved from Eq. (8) [5]. For LBGK computation, it is highly desirable to have lattices with minimal number of smallest velocities, yet with highest degree of precision. To obtain such lattices, we consider the vectors in a size-m Cartesian gird, i.e., $\boldsymbol{\xi}_i = c\boldsymbol{e}_i$, where c is the *lattice constant*, and $\{\boldsymbol{e}_i\}$ all vectors with integer components in the range of $[-m, m]$. The number of all such vectors is $d = (2m+1)^D$, where D is the dimensionality. For symmetry reasons, all weights in the same symmetry group must be the same. On substituting $\boldsymbol{\xi}_i = c\boldsymbol{e}_i$ into Eq. (8), we obtain a set of linear equations about the weights with the coefficients being polynomials in c. The number of equations is determined by Q and the number of variables by the size of the lattice m. Depending on these two numbers and the value of the lattice constant, Eq. (8) may or may not have a solution. For a degree of precision up to 9, which recovers moments up to the fourth order, we were able to find solutions within $m = 3$ lattice. When solutions do exist, they are found to form a linear space in the parameter space spanned by the weight vector. We shall discuss the details of the solutions in the following sections.

III. TWO-DIMENSIONAL LATTICES

In Table I the vectors and the symmetry groups are listed up to $m=3$. In the two-dimensional (2D) case, there are ten symmetry groups and therefore ten weights. Define the vector $\bar{w}=(w_1,\cdots,w_{10})$. Substituting the vectors in Table I into Eq. (8) up to $Q=8$, a set of linear equations in the form of

$$M\bar{w}^T=(1,0,\ldots,0)^T \tag{9}$$

are obtained, where the matrix M is given in the following:

$$\begin{bmatrix} 1 & 4 & 4 & 4 & 8 & 4 & 4 & 8 & 8 & 4 \\ -1 & 2c^2-4 & 4c^2-4 & 8c^2-4 & 4(5c^2-2) & 4(4c^2-1) & 18c^2-4 & 8(5c^2-1) & 4(13c^2-2) & 4(9c^2-1) \\ 0 & -1 & 2c^2-2 & -4 & 2(8c^2-5) & 8(4c^2-1) & -9 & 4(9c^2-5) & 2(72c^2-13) & 18(9c^2-1) \\ 0 & 0 & c^2-3 & 6 & 4(2c^2-3) & 4(4c^2-9) & 36 & 18(c^2+1) & 12(6c^2-11) & 9(9c^2-19) \\ 0 & 0 & -1 & 4c^2 & 2(c^2-4) & -16(c^2+1) & 54c^2 & 18(4c^2-1) & -82c^2-72 & -81-216c^2 \\ 0 & 0 & 0 & -1 & 2(c^2-1) & 2(4c^2-1) & -6 & 12(c^2-1) & 66c^2-14 & 12(9c^2-1) \\ 0 & 0 & 0 & 0 & c^2-3 & 4(4c^2-3) & 0 & 6(c^2-3) & 3(59c^2-33) & 162(3c^2-1) \\ 0 & 0 & 0 & 0 & 114 & 2A & 0 & B & 2C & 27D \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2(c^2-1) & 2(4c^2-1) & 2(9c^2-1) \end{bmatrix} \tag{10}$$

where

$$A=228+507c^2-741c^4+103c^6-4c^8 \tag{11a}$$

$$B=684-2415c^2+1470c^4-140c^6+5c^8 \tag{11b}$$

$$C=1881+1254c^2-5952c^4+956c^6-38c^8 \tag{11c}$$

$$D=228+547c^2-1486c^4+228c^6-9c^8. \tag{11d}$$

Note that first, due to the symmetry of the lattice vectors, Eq. (8) is automatically satisfied at all odd orders. Second, in Eq. (10) there are nine equations for the eleven variables, $w_1,\ldots,w_{10}$ and the lattice constant c. Specifically, the first equation is from Eq. (8) at $n=0$; the second equation is by $n=2$; the third and fourth by $n=4$; the fifth and sixth by $n=6$; and the seventh, eighth and ninth by $n=8$. Therefore, solutions of the first four equations give fifth degree quadratures, the one employed by the standard LBGK. Solutions of the first six equations give seventh degree quadratures and solutions of all nine equations give ninth degree quadratures.

At the lowest order, the first four equations define the fifth-order quadratures in the athermal LB models with approximate Galilean invariance [10]. If only the $m=1$ lattices are allowed, i.e., $w_i=0$ for $i=4,\ldots,10$, only the upper-left 4×3 submatrix needs to be considered, and the only possible solution is $c^2=3$ and $w_1=4/9$, $w_2=1/9$, and $w_3=1/36$, which is the classic D2Q9 model.

At the next order, the general solutions of seventh-order quadratures are given by the first six equations in Eq. (9)

$$w_1=1-\frac{7}{3c^6}+\frac{23}{6c^4}-\frac{49}{18c^2}+36w_6+80w_8+512w_9+976w_{10} \tag{12a}$$

$$w_2=\frac{19}{16c^6}-\frac{77}{48c^4}+\frac{3}{4c^2}-24w_6-50w_8-318w_9-594w_{10} \tag{12b}$$

$$w_3=\frac{5c^2-6}{12c^6}+16w_6+30w_8+192w_9+351w_{10} \tag{12c}$$

$$w_4=\frac{-1}{4c^6}+\frac{7}{24c^4}-\frac{3}{40c^2}+6w_6+12w_8+64w_9+108w_{10} \tag{12d}$$

TABLE I. Two-dimensional lattice and quadrature. For each symmetry group, a typical lattice vector and the number of vectors in the group, p, are given. Groups of different sizes ($m=0,1,2,3$) are listed in separate sections. Following the previous naming convention [5], each quadrature is named with its dimensionality D, the degree of precision, N, and the number of points, d, as $E_{D,N}^{d}$.

Group	Vector	p	$E_{2,7}^{17}$ $c^2=(5\pm\sqrt{10})/3$
1	(0,0)	1	$2(95\mp4\sqrt{10})/405$
2	(0,1)	4	$3(-5\pm4\sqrt{10})/200$
3	(1,1)	4	$3(50\mp13\sqrt{10})/800$
4	(0,2)	4	
5	(1,2)	8	
6	(2,2)	4	
7	(0,3)	4	$295\mp92\sqrt{10}/16200$
8	(1,3)	8	
9	(2,3)	8	
10	(3,3)	4	$130\mp41\sqrt{10}/64800$

$$w_5 = \frac{3-c^2}{48c^6} - 4w_6 - 6w_8 - 33w_9 - 54w_{10} \tag{12e}$$

$$w_7 = \frac{4c^4 - 15c^2 + 15}{720c^6} - 2(w_8 + w_9 + w_{10}). \tag{12f}$$

A few observations can be made. First, it is immediately clear from Eq. (12f) that there is no seventh degree lattice within $m=2$ because $4c^4-15c^2+15$ is positive definite for any real c so that w_7, w_8, w_9, and w_{10} cannot all be zero together.

Second, Eq. (12), which contain infinite number of solutions, has the structure of a four-dimensional linear space. Namely, the weight vector can be written as

$$\bar{w} = \bar{w}_0 + \bar{\omega} W, \tag{13}$$

where $\bar{w}_0$ is a particular solution, W a 4×10 matrix, and $\bar{\omega} = (\omega_1, \ldots, \omega_4)$ an arbitrary vector. We can therefore eliminate any four groups and still have a solution for any arbitrary lattice constant. The lattice constant could be further chosen so that one of the remaining six weights is zero, leaving the total number of nonzero weights to 5. Thus, a seventh degree quadrature must include at least five of the symmetry groups. Choosing the five least populous groups, i.e., group 1 with any four of the six groups with four velocities, the minimal number of velocities is therefore $1+4\times 4=17$. The $E_{2,7}^{17}$ quadrature in Ref. [5], which is also given as the D2V17 model in Ref. [8], is such an example. The two D2V25 lattices given in the same work employ more velocities while having the same *degree of precision* as quadratures.

Third, restricting the velocities to those with components $\{0, \pm 1, \pm 3\}$, we have the D2Q25ZOT (zero-one-three) lattice [19] which requires $w_4=w_5=w_6=w_9=0$. From the new constraints $w_4=w_5=0$, we have $3c^4-10c^2+5=0$, or $c^2 = (5\pm\sqrt{10})/3$, and

$$w_8 + 9w_{10} = \frac{3-c^2}{288c^6}. \tag{14}$$

We are left with one free parameter and the weights of the D2Q25ZOT form a 1D linear space. Using the extra degree of freedom to eliminate the most populous group 8, we have a pair of 17-velocity ZOT quadratures which are also minimal. The weights and the corresponding lattice constants are shown in Table I. Note that the weights are all positive only if the upper sign is taken.

Finally we note that solutions with negative weights result in negative components in the distribution function. This is undesirable because it not only contradicts with the conventional probabilistic definition of the distribution function, but also cause numerical instabilities in simulations (cf., e.g., [23]). With the positivity constrain, the problem of finding the minimal quadrature formally reduces to a problem of Linear Programming of finding the vector $\bar{w}$ which minimize the number of points under equality constrain (12) and the inequality constrains $w_i \geq 0$.

All 9th order quadratures within $m=3$ are given by solving the entire Eq. (9) for the eleven variables. It is found that the only real positive solution for the lattice constant c is

$$c = \frac{1}{6}\sqrt{49 - \frac{119 + (469+252\sqrt{30})^{2/3}}{(469+252\sqrt{30})^{1/3}}} \cong 1.196\,98. \tag{15}$$

Under this condition, Eq. (9) reduces to [24]

$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \\ w_6 \\ w_7 \\ w_8 \end{bmatrix} + \begin{bmatrix} 240 & 1040 \\ -170 & -720 \\ 120 & 495 \\ 56 & 216 \\ -39 & -144 \\ 12 & 36 \\ -6 & -16 \\ 4 & 9 \end{bmatrix} \begin{bmatrix} w_9 \\ w_{10} \end{bmatrix} = \begin{bmatrix} 0.233\,15 \\ 0.107\,30 \\ 0.057\,66 \\ 0.014\,20 \\ 0.005\,35 \\ 0.001\,01 \\ 0.000\,24 \\ 0.000\,28 \end{bmatrix}, \tag{16}$$

which defines a two-dimensional subspace in a ten-dimensional linear space. By eliminating any two of the three most populous groups 5, 8, and 9, we obtain three 33-velocity quadratures which all have some negative weights. The all-positive ninth-order 37-point quadrature D2V37 in Ref. [8] is therefore minimal within $m=3$.

IV. THREE-DIMENSIONAL LATTICES

The same principle applies in 3D with slightly different results. Given in Table II are all lattice vectors within $m=3$. Note there are 20 symmetry groups in 3D. On substituting the vectors into Eq. (8), 11 linear equations of the form of Eq. (9) are obtained. As the full detail of the matrix is too lengthy to be given here, we shall discuss the solutions in separate cases below.

For the fifth-order quadrature [$Q=5$ in Eq. (8)], there are four independent equations. On restricting the lattice to $m=1$, i.e., setting $w_i=0$ for $i=5,\cdots,20$, and after some manipulations, they are

$$\begin{bmatrix} 1 & 6 & 12 & 8 \\ 0 & 2c^2 & 8c^2 & 8c^2 \\ 0 & c^2-3 & 4(c^2-3) & 4(c^2-3) \\ 0 & -1 & 2(c^2-2) & 4(c^2-1) \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}. \tag{17}$$

It is easy to see that if and only if $c^2=3$, the equations above have the solution,

$$w_1 = \frac{1}{3} - 8w_4 \tag{18a}$$

$$w_2 = \frac{1}{18} + 4w_4 \tag{18b}$$

$$w_3 = \frac{1}{36} - 2w_4, \tag{18c}$$

of which the well-known D3Q15, D3Q19 and D3Q27 lattices are all special cases.

For the seventh-order quadratures, there are seven equations in Eq. (9). The general solution is

TABLE II. Three-dimensional lattice and quadratures. For each symmetry group, a typical lattice vector and the number of vectors in the group, p, are given. Groups of different sizes ($m=0,1,2,3$) are in separate sections. Following the previous naming convention [5], each quadrature is named with its dimensionality D, the degree of precision, N, and the number of points, d, as $E_{D,N}^{d}$.

Group	Vector	p	$E_{3,9}^{103}$ $c^2=1.43276$
1	(0,0,0)	1	3.2633×10^{-2}
2	(0,0,1)	6	9.7657×10^{-2}
3	(0,1,1)	12	
4	(1,1,1)	8	2.8098×10^{-2}
5	(0,0,2)	6	1.0452×10^{-3}
6	(0,1,2)	24	5.7053×10^{-3}
7	(0,2,2)	12	6.1194×10^{-4}
8	(1,1,2)	24	
9	(1,2,2)	24	
10	(2,2,2)	8	1.5596×10^{-4}
11	(0,0,3)	6	2.8444×10^{-4}
12	(0,1,3)	24	
13	(0,2,3)	24	
14	(0,3,3)	12	
15	(1,1,3)	24	1.3070×10^{-4}
16	(1,2,3)	48	
17	(1,3,3)	24	
18	(2,2,3)	24	
19	(2,3,3)	24	
20	(3,3,3)	8	1.2232×10^{-6}

$$w_1 = 1 - \frac{27}{4c^6} + \frac{8}{c^4} - \frac{49}{12c^2} + 108w_7 + 72w_8 + 576w_9 + 720w_{10} + 240w_{12} + 1536w_{13} + 2928w_{14} + 672w_{15} + 5232w_{16} + 8256w_{17} + 6720w_{18} + 166\,80w_{19} + 116\,80w_{20} \tag{19a}$$

$$w_2 = \frac{41}{16c^6} - \frac{115}{48c^4} + \frac{3}{4c^2} - 4(12w_7 + 10w_8 + 71w_9 + 88w_{10} + 25w_{12} + 159w_{13} + 297w_{14} + 75w_{15} + 582w_{16} + 886w_{17} + 774w_{18} + 1884w_{19} + 1323w_{20}) \tag{19b}$$

$$w_3 = \frac{-3}{4c^6} + \frac{5}{12c^4} + 16w_7 + 22w_8 + 128w_9 + 160w_{10} + 30w_{12} + 192w_{13} + 351w_{14} + 112w_{15} + 876w_{16} + 1248w_{17} + 1280w_{18} + 3030w_{19} + 2160w_{20} \tag{19c}$$

$$w_4 = \frac{1}{8c^6} - 12w_8 - 48w_9 - 64w_{10} - 27w_{15} - 216w_{16} - 243w_{17} - 432w_{18} - 972w_{19} - 729w_{20} \tag{19d}$$

$$w_5 = \frac{-3}{8c^6} + \frac{1}{3c^4} - \frac{3}{40c^2} + 4(3w_7 + w_8 + 8w_9 + 7w_{10} + 6w_{12} + 32w_{13} + 54w_{14} + 12w_{15} + 78w_{16} + 120w_{17} + 72w_{18} + 173w_{19} + 108w_{20}) \tag{19e}$$

$$w_6 = \frac{c^2-3}{48c^6} - (4w_7 + 2w_8 + 10w_9 + 8w_{10} + 6w_{12} + 33w_{13} + 54w_{14} + 12w_{15} + 80w_{16} + 120w_{17} + 74w_{18} + 174w_{19} + 108w_{20}) \tag{19f}$$

$$w_{11} = \frac{4c^4 - 15c^2 + 15}{720c^6} - 4(w_{12} + w_{13} + w_{14} + w_{15} + 2w_{16} + 2w_{17} + w_{18} + 2w_{19} + w_{20}) \tag{19g}$$

It is immediately clear that no solution exists within $m=2$ as it would require $w_i=0$ for $i=11,\cdots,20$, which contradicts with the last equation.

Parallel to the discussion in 2D, the general solutions above form a 13-dimensional linear space. Using the extra degree of freedom of c, fourteen of the twenty weights could be zero. Therefore, a seventh-order quadrature must include at least six of the symmetry groups in Table II. The total population of the six least populous groups defines the *lower bound* on the number of velocities. Unfortunately setting the corresponding weights to zero in Eq. (19) results in a conflict, which implies that at least one of the groups with twelve velocities has to be included. Therefore the 39-point quadrature $E_{3,7}^{39}$ of Ref. [5] is minimal. As a comparison, the D3V59 lattice [16] uses more and larger velocities while having the same degree of precision as a quadrature.

The three-dimensional ZOT lattices [19] can be easily verified as a special case of Eq. (19). Setting $w_i=0$ in Eq. (19) for $i\in\{5-10,13,16,18,19\}$, the conditions $w_5=w_6=0$ yield $3c^4-10c^2+5=0$, or $c^2=(5\pm\sqrt{10})/3$, and

$$w_{12} + 9w_{14} + 2w_{15} + 20w_{17} + 18w_{20} = \frac{3-c^2}{288c^6} \tag{20}$$

where the two values of c correspond to the "higher-T_0" and the "lower-T_0" versions of the ZOT lattice. The weights form a four-dimensional linear space. After eliminating four most populous groups, i.e., groups 12, 14, 15, and 17, we arrive at the two D3Q41 lattices which are the minimal ZOT lattices but unlike in 2D, not minimal overall.

The ninth-order quadratures are given by the entire set of eleven equations. Similar to the 2D situation, Eq. (9) has solution if and only if c takes the value given by Eq. (15). In that case, the solutions form a ten-dimensional subspace of the 20-dimensional linear space,

$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \\ w_6 \\ w_7 \\ w_8 \\ w_{11} \\ w_{12} \end{bmatrix} + \begin{bmatrix} 216 & 648 & 720 & 3120 & 240 & 4512 & 12\,096 & 10\,104 & 36\,864 & 35\,408 \\ -132 & -384 & -340 & -1440 & -140 & -2464 & -6232 & -5672 & -20\,192 & -19\,404 \\ 80 & 224 & 120 & 495 & 80 & 1260 & 2880 & 3072 & 10572 & 10224 \\ -48 & -128 & 0 & 0 & -45 & -576 & -1053 & -1584 & -5184 & -5103 \\ 24 & 60 & 112 & 432 & 24 & 480 & 1296 & 888 & 3136 & 2808 \\ -14 & -32 & -39 & -144 & -12 & -208 & -504 & -414 & -1392 & -1260 \\ 2 & 2 & 12 & 36 & 0 & 24 & 72 & 26 & 96 & 72 \\ 8 & 16 & 0 & 0 & 6 & 66 & 108 & 168 & 513 & 486 \\ 0 & 0 & -12 & -32 & -4 & -32 & -72 & -28 & -96 & -68 \\ 0 & 0 & 4 & 9 & 2 & 10 & 20 & 8 & 26 & 18 \end{bmatrix} \begin{bmatrix} w_9 \\ w_{10} \\ w_{13} \\ w_{14} \\ w_{15} \\ w_{16} \\ w_{17} \\ w_{18} \\ w_{19} \\ w_{20} \end{bmatrix} = \begin{bmatrix} 0.208\,37 \\ -0.004\,26 \\ 0.057\,89 \\ -0.003\,98 \\ 0.016\,97 \\ -0.002\,39 \\ 0.001\,01 \\ 0.003\,87 \\ -0.000\,32 \\ 0.000\,28 \end{bmatrix}. \tag{21}$$

Special cases of the general solution can be found to minimize the number of velocities. However, excluding the ten most populous groups (those with 24 velocities or more) causes a conflict. The lower bound on the number of velocities is therefore 91, the smallest total population when one group with 24 velocities is included. Lattices of 91 velocities are indeed obtained but all with some of the weights negative. All-positive lattices are also obtained using a linear-programming solver. Of particular interests are the 103-velocity lattice given in Table II which is the next smallest velocity set after 91, and the 121-velocity lattice [9,10], both of which are two orders more accurate than the ZOT lattices within the same velocity bound. The existence of 91-velocity ninth-order quadrature cannot be analytically excluded at this time. By using velocities from the next level, more ninth-order lattices can be obtained such as the D3V107 lattice [16].

V. DISCUSSIONS AND CONCLUSIONS

Summarizing, we give the general solutions of Cartesian LBGK lattices in both two and three dimensions with the focus on the comprehensiveness and minimality of the lattices and the connections among various ways of obtaining them. The solutions have the mathematical structure of linear subspaces in the linear space spanned by the quadrature weights. All the Cartesian LBGK lattices that we are aware of are special cases of the general solutions with the apparent exception of the D3Q13 model which is not a BGK type model [25]. Using the general solutions, lower bounds on the number of velocities for the seventh- and ninth-order lattices are established (17 and 37 in 2D, 39 and 91 in 3D) and minimal or near-minimal lattices are identified in both dimensions. The resulting LBGK models are adequate for the complete recovery of the Navier-Stokes momentum and thermal equations respectively.

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