Theory of the lattice Boltzmann equation: Symmetry properties of discrete velocity sets

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The lattice Boltzmann equation replaces continuous particle velocity space by a finite set; the velocity distribution function then varies over a finite-dimensional vector space instead of over an infinite-dimensional function space. The number of linearly independent moments of the distribution function in a lattice Boltzmann model cannot exceed the number of velocities; finite dimensionality therefore necessarily induces linear dependences among the moments that do not exist in a continuous theory. Given a finite velocity set, it is important to know which moments are free of these dependences. Elementary group theory is applied to the solution of this problem. It is found that decomposing the velocity set into subsets that transform among themselves under an appropriate symmetry group makes it straightforward to uncover linear dependences among the moments. The construction of some standard two- and three-dimensional models is reviewed from this viewpoint, and procedures for constructing higher-dimensional models are suggested.

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I. INTRODUCTION

A guiding principle of this series of papers is the formulation of the lattice Boltzmann equation (LBE) as a discrete kinetic theory [1–10]. In kinetic theory, moments of the distribution function $f(\boldsymbol{x},\boldsymbol{\xi},t)$ over the space of velocities $\boldsymbol{\xi}$ are the components of tensors of various ranks [11,12] that define continuum fluid properties like mass, momentum, energy, stress, and heat flux. Analogous moments can be formed in the discrete setting of the lattice Boltzmann equation; however, since the number of linearly independent moments cannot exceed the number of velocities, discreteness permits linear dependences that do not exist in the continuous case [13].

Thus, in kinetic theory, the number of linearly independent moments of order n,

$$\mathsf{M}(\boldsymbol{x},t) = \int d\boldsymbol{\xi} \underbrace{\boldsymbol{\xi}\cdots\boldsymbol{\xi}}_{n\ \text{times}} f(\boldsymbol{x},\boldsymbol{\xi},t), \tag{1}$$

is equal to the number of linearly independent products $\boldsymbol{\xi}\cdots\boldsymbol{\xi}$ in the integrand—namely, $(n+1)(n+2)/2$ in three dimensions and $(n+1)$ in two dimensions. But in a *discrete* kinetic theory, in which the integral over continuous velocity space $\boldsymbol{\xi}$ in Eq. (1) is replaced by a sum over a finite velocity set C with N elements,

$$\mathsf{M}(\boldsymbol{x},t) = \sum_{\boldsymbol{c}_i\in\mathsf{C}} \underbrace{\boldsymbol{c}_i\cdots\boldsymbol{c}_i}_{n\ \text{times}} f_i(\boldsymbol{x},t) \tag{2}$$

the factor $f_i(\boldsymbol{x},t)$ restricts the number of linearly independent moments to at most N. Therefore, if $N<(n+1)(n+2)/2$, the tensor defined in the discrete theory by Eq. (2) necessarily has fewer independent components than its continuous counterpart defined by Eq. (1). Such a reduction remains possible due to linear dependences even if $N\geq(n+1)(n+2)/2$. Whenever a tensor in a discrete theory has fewer independent components than its continuous counterpart, we will say that the tensor is *incomplete* in this discrete theory; if it has the same number, we will say that it is *complete*.[1]

Incomplete tensors in a discrete model are artifacts without continuous analogs; a fundamental problem in discrete kinetic theory is therefore given a finite velocity set $\mathsf{C}:=\{\boldsymbol{c}_i\}$ to determine what tensors are complete. The purpose of this paper is to develop a systematic approach to solve this problem. The approach is based on the observation that the discrete velocity set $\{\boldsymbol{c}_i\}$ is not an arbitrary collection, but is chosen to be as symmetric as possible so that the model can mimic the physical isotropy of the fluid. In particular, two-dimensional models typically are based on a discrete velocity set with the symmetry of a square: that is, it is invariant under a group of transformations of two-dimensional $\boldsymbol{\xi}$ space that map the set of four velocities $\{(\pm1,\pm1)\}$ into itself, and three-dimensional models are typically based on a velocity set with the symmetry of a cube: that is, it is invariant under a group of transformations of three-dimensional $\boldsymbol{\xi}$ space that map the analogous set of eight velocities $\{(\pm1,\pm1,\pm1)\}$ into itself.

It is natural to exploit the symmetry of the configuration of discrete velocities by applying the elementary representation theory of finite groups (cf. [14,15]). Although models can and have been constructed case by case using elementary methods, group theory offers the advantages of a systematic and unified approach. We do not claim that group theory results in a "better" way to construct models, in the sense of being faster, easier to formulate, or even easier to understand. We only contend that group theory provides a natural approach that reveals some problems common to constructing any discrete model, which can be hidden by lengthy al-

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[1]This definition will be applied, for example, to a *trace-free* second-rank tensor; such a tensor is complete in three dimensions if it has five components. Completeness of a second-rank tensor does not require that it have the maximum number, 6, independent components. This convention will apply to tensors of arbitrary rank.

gebra, even (or perhaps especially) if the algebra is done symbolically. We note that group theory has also been used to study lattice-gas cellular automata [16–22] and lattice Boltzmann models [23–25] from a different perspective. The content of this paper is limited to the *kinematics* of the description of tensors by finite discrete velocity models; a tensor need not be well described *dynamically* in a model in which it is complete: this issue will be discussed at the end of the paper.

The outline of the paper is as follows. We shall first review elementary group theory and its application to simple discrete velocity sets in three dimensions based on the vertices, edges, and faces of a cube. The group theoretical analysis will be used to study models D3Q6, D3Q13, D3Q15, D3Q19, and D3Q27. (Here, the standard notation D*d*Q*q* is used to denote a *q*-velocity model in *d*-dimensional space.) Some preliminary discussion of a D3Q51 model will be given. We shall also discuss some two-dimensional models. It will be shown that expressing the models in terms of irreducible representations (cf. [14,15,26]) of the group of symmetries of a cube or a square can help answer basic questions about the kinematics of discrete models. Brief discussions are then given of the role of the choice of symmetry group and of the role of higher-order moments in discrete hydrodynamics.

II. DECOMPOSITION INTO IRREDUCIBLE REPRESENTATIONS IN THREE DIMENSIONS

The formulation of lattice Boltzmann models begins with a discrete velocity set $\mathsf{C}=\{\boldsymbol{c}_i\}$ chosen from a lattice $\delta_x\mathbb{Z}^D$ with lattice constant δ_x in continuous D-dimensional velocity space $\boldsymbol{\xi}$. In three dimensions, the highest symmetry possible for the set C is the symmetry of a cube (cf. [26]). Since a model with any less symmetry cannot be satisfactory, this symmetry will be imposed on all velocity sets C at the outset. We will describe this symmetry by the group of 24 *rotations* of the cube. Adding inversions leads to the complete group of 48 symmetries; however, it will appear that the main ideas can be explained and understood more simply using the smaller group.

The distribution function is a finite sum

$$f(\boldsymbol{x},\boldsymbol{\xi},t) := \sum_{\boldsymbol{c}_i\in\mathsf{C}} f_i(\boldsymbol{x},t)\,\delta(\boldsymbol{\xi}-\boldsymbol{c}_i), \tag{3}$$

where $f_i(\boldsymbol{x},t)$ is the discrete particle distribution function associated with particles with discrete velocity $\boldsymbol{c}_i$ [1,2]. It will sometimes be convenient to write the distribution function as a function of the velocities in the finite-dimensional vector space spanned by the set C as

$$f(\boldsymbol{x},\boldsymbol{c},t) := \sum_{\boldsymbol{c}_i\in\mathsf{C}} f_i(\boldsymbol{x},t)\hat{\boldsymbol{c}}_i, \tag{4}$$

where $\hat{\boldsymbol{c}}_i$ assigns unit particle population to the velocity $\boldsymbol{c}_i$ and zero to all other velocities.

The multiple-relaxation-time (MRT) formalism of d'Humières *et al.* [5,13,27] models the collision process through the relaxation of moments, which therefore play a central role in the formulation. Moments of the distribution function f are defined in terms of polynomials chosen from a set $\{p_j(\boldsymbol{\xi})\}$ by

$$\mathsf{M}_j(\boldsymbol{x},t) = \int d\boldsymbol{\xi}\, f(\boldsymbol{x},\boldsymbol{\xi},t)p_j(\boldsymbol{\xi}) = \sum_{\boldsymbol{c}_i\in\mathsf{C}} f_i(\boldsymbol{x},t)p_j(\boldsymbol{c}_i). \tag{5}$$

Thus, values of the moments are determined by linear combinations of rows of the matrix:

$$A_{ij} = \langle p_j|\boldsymbol{c}_i\rangle := \int d\boldsymbol{\xi}\;\delta(\boldsymbol{\xi}-\boldsymbol{c}_i)p_j(\boldsymbol{\xi}) = p_j(\boldsymbol{c}_i), \tag{6}$$

where the bra-ket notation is extended by linearity to linear combinations of polynomials and velocities.

The number of linearly independent moments is the rank of the matrix A in Eq. (6) when p_j varies over the chosen set of homogeneous polynomials and $\boldsymbol{c}_i$ varies over the set C. The rank can certainly be found by straightforward linear algebra; however, useful simplifications result if the matrix A is evaluated after expressing both $\{\boldsymbol{c}_i\}$ and $\{p_j(\boldsymbol{\xi})\}$, regarded as bases of vector spaces on which the group of rotations of the cube acts as a group of linear transformations, in bases $\{\tilde{\boldsymbol{c}}_i\}$ and $\{\tilde{p}_j(\boldsymbol{\xi})\}$ consisting of quantities that transform by *irreducible representations* [14,15,26] of the group of rotations of the cube. The resulting matrix will be denoted by $\tilde{\mathsf{A}}$. The irreducible representations are the representations of the lowest dimension from which all possible representations can be constructed; we refer to elementary texts (e.g., [14,15,26]) for details. Fundamental orthogonality properties imply that $\tilde{A}_{ij}=\langle\tilde{p}_j|\tilde{\boldsymbol{c}}_i\rangle=0$ whenever $\tilde{p}_j$ and $\tilde{\boldsymbol{c}}_i$ belong to different irreducible representations. Thus, $\tilde{\mathsf{A}}$ consists of blocks $\tilde{A}_{ij}$ in which the indices i and j vary over vectors transforming by the same irreducible representation. These blocks are $dn\times dn$ if there are n occurrences of an irreducible representation of dimension d; since these blocks are much smaller than the original matrix A, the computation of the rank is greatly simplified.

The irreducible representations of the group of 24 rotations of the cube are exhibited in the following [14,15,26]:

Repr.	Polynomials
Γ_1	1
Γ_1'	xyz
Γ_2	$\{(x^2-y^2),(y^2-z^2),(z^2-x^2)\} := \{*(x^2-y^2)\}$
Γ_3	$\{xy,yz,zx\} := \{*xy\}$
Γ_3'	$\{x,y,z\} := \{*x\}$

(7)

The notation $*p(x,y,z)$ will be used henceforth to indicate the additional polynomials obtained from $p(x,y,z)$ by cyclic permutation of x, y, and z. The notation x, y, and z and index notation x_1, x_2, and x_3 will both be used as convenient to denote the components of the particle velocity $\boldsymbol{\xi}$: no ambiguity is possible because configuration space $\boldsymbol{x}$ plays no role in this paper. In the table above, for each representation Γ_n, the subscript n indicates its dimension and a set of n linearly independent polynomials is given which transforms irreducibly according to Γ_n. Representations of the same dimension are distinguished by primes. Only two of the polynomials listed for Γ_2 are linearly independent. We prefer this symmetric notation to making a (necessarily) unsymmetric choice of a basis for the space on which this representation is defined.

A. Discrete velocity sets

The smallest discrete velocity sets invariant under the group of rotations of the cube are formed from the vectors describing the edges E, vertices V, faces F, and the center O of a cube. Explicitly, these sets are

$$\text{12 edges}\quad \mathsf{E}\quad \{(\pm 1, \pm 1,0),(\pm 1,0, \pm 1),(0, \pm 1, \pm 1)\},$$

$$\text{8 vertices}\quad \mathsf{V}\quad \{(\pm 1, \pm 1, \pm 1)\},$$

$$\text{6 faces}\quad \mathsf{F}\quad \{(\pm 1,0,0),(0, \pm 1,0),(0,0, \pm 1)\},$$

$$\text{1 center}\quad \mathsf{O}\quad \{(0,0,0)\}, \tag{8}$$

where, in the interest of simplicity, the lattice constant δ_x is taken to be the unit of length. These sets are bases of finite-dimensional vector spaces on which the group of rotations of the cube acts as a group of linear transformations. To simplify the notation, these vector spaces and the representations of the rotation group of the cube which they carry will also be denoted by the letters E, V, F, and O, even though, strictly speaking, the representations are sets of linear transformations (or matrices) defined over these vector spaces.

Routine calculations give the decompositions into irreducible representations

$$\mathsf{E} = \Gamma_1 \oplus \Gamma_2 \oplus 2\Gamma_3 \oplus \Gamma_3', \tag{9a}$$

$$\mathsf{V} = \Gamma_1 \oplus \Gamma_1' \oplus \Gamma_3 \oplus \Gamma_3', \tag{9b}$$

$$\mathsf{F} = \Gamma_1 \oplus \Gamma_2 \oplus \Gamma_3', \tag{9c}$$

$$\mathsf{O} = \Gamma_1. \tag{9d}$$

The explicit linear combinations of velocities that occur in these decompositions are listed in the Appendix.

The meaning of these decompositions is very simple. Consider, for example, the decomposition of F: if we have a linear combination of these velocities $\Sigma a_i \boldsymbol{c}_i$, introducing the basis given in Eq. (A1), which we write as $\tilde{\boldsymbol{c}}^1$ for Γ_1, $\tilde{\boldsymbol{c}}_1^2$ and $\tilde{\boldsymbol{c}}_2^2$ for Γ_2, and $\tilde{\boldsymbol{c}}_1^3$, $\tilde{\boldsymbol{c}}_2^3$, and $\tilde{\boldsymbol{c}}_3^3$ for Γ_3', we have

$$\sum_{\boldsymbol{c}_i \in \mathsf{F}} a_i \hat{\boldsymbol{c}}_i = a^1 \tilde{\boldsymbol{c}}^1 + a_1^2 \tilde{\boldsymbol{c}}_1^2 + a_2^2 \tilde{\boldsymbol{c}}_2^2 + a_1^3 \tilde{\boldsymbol{c}}_1^3 + a_2^3 \tilde{\boldsymbol{c}}_2^3 + a_3^3 \tilde{\boldsymbol{c}}_3^3. \tag{10}$$

Whereas arbitrary rotations of the sphere mix all of the coefficients a_i, the coefficient a^1 is invariant under all rotations of the cube, the coefficients a_i^3, $i=1,2,3$, transform among themselves according to the irreducible representation Γ_3', and the coefficients a_i^2 transform according to Γ_2.

The absence of the representation Γ_3 in the decomposition of F in Eq. (9c) suggests that the three polynomials $*\{xy\}$ that transform among themselves by Γ_3 according to Eq. (7) must vanish in the set F. Similarly, the absence of the representation Γ_2 in the decomposition of V implies that $*\{x^2 - y^2\}$ vanish on V. Although these results are both obvious, it will be shown that group theory can help uncover less obvious linear relations.

Turning to the velocity sets that are commonly used to construct LBE models, consider the D3Q13 [28], D3Q15, D3Q19, and D3Q27 models. The decompositions into irreducible representations of the representations of the group of rotations of the cube acting on the vector spaces generated by these velocity sets are perhaps best given in a table, which is easily obtained from Eqs. (9a)–(9d):

Model	Velocity set	Decomposition
D3Q13	$\mathsf{E} \cup \mathsf{O}$	$2\Gamma_1 \oplus \Gamma_2 \oplus 2\Gamma_3 \oplus \Gamma_3'$
D3Q15	$\mathsf{F} \cup \mathsf{V} \cup \mathsf{O}$	$3\Gamma_1 \oplus \Gamma_1' \oplus \Gamma_2 \oplus \Gamma_3 \oplus 2\Gamma_3'$
D3Q19	$\mathsf{F} \cup \mathsf{E} \cup \mathsf{O}$	$3\Gamma_1 \oplus 2\Gamma_2 \oplus 2\Gamma_3 \oplus 2\Gamma_3'$
D3Q21	$\mathsf{E} \cup \mathsf{V} \cup \mathsf{O}$	$3\Gamma_1 \oplus \Gamma_1' \oplus \Gamma_2 \oplus 3\Gamma_3 \oplus 2\Gamma_3'$
D3Q27	$\mathsf{E} \cup \mathsf{V} \cup \mathsf{F} \cup \mathsf{O}$	$4\Gamma_1 \oplus \Gamma_1' \oplus 2\Gamma_2 \oplus 3\Gamma_3 \oplus 3\Gamma_3'$

(11)

The theoretically possible model D3Q21 is given in the interest of completeness.

B. Polynomials

We next consider the polynomials $\{p_j(\boldsymbol{\xi})\}$ that generate the moments. The rotations of the cube form a group of linear transformations of the continuous vector variable $\boldsymbol{\xi}$ and, by obvious extension, a group of linear transformations of homogeneous polynomials in the components of $\boldsymbol{\xi}$. We will again require the decomposition of these representations into irreducible representations.

Denote by P^n the set of all homogeneous polynomials in (x,y,z) of degree n. It is obvious that any constant P^0 is a rotational invariant and therefore transforms as Γ_1. According to Eq. (7), linear polynomials P^1 transform irreducibly as Γ_3'. For quadratic polynomials, a new possibility arises: any quadratic polynomial is a linear combination of

$$r^2 \equiv x^2 + y^2 + z^2, \tag{12}$$

an invariant [also of the group of all rotations of space SO(3)] that transforms as Γ_1, and a remainder. This decomposition also occurs in the continuous case, where it is reflected in the occurrence of the (scalar) pressure as the trace of the stress tensor. This decomposition can be written as

$$P^2 = r^2 P^0 \oplus P^{2,0}, \tag{13}$$

where $P^{2,0}$ denotes the set $\{a_{ij}x_i x_j | a_{kk}=0\}$ of quadratics with a trace-free coefficient matrix. According to Eqs. (9a)–(9d), the representation of the group of rotations of the cube on $P^{2,0}$ splits into the sum

$$P^{2,0} = \Gamma_2 \oplus \Gamma_3, \tag{14}$$

so that finally

$$P^2 = \Gamma_1 \oplus \Gamma_2 \oplus \Gamma_3. \tag{15}$$

For cubic polynomials, we note first that the product of r^2 and a linear polynomial evidently transforms by the irreducible representation Γ_3'. Separating this contribution, we obtain an analog of Eq. (13):

$$P^3 = r^2 P^1 \oplus P^{3,0}. \tag{16}$$

The first term corresponds to the possibility of generating a vector from a symmetric third-rank tensor a_{imn} by the contraction $a_i = \delta_{mn} a_{imn}$. A familiar physical example is the generation of the heat flux vector from the stress flux tensor. The remaining seven polynomials $P^{3,0}$ define an irreducible representation of SO(3). Equations (13) and (16) illustrate how the trace operation is used to construct irreducible representations of SO(3) [29].[2]

The representation of the group of rotations of the cube on $P^{3,0}$ splits into the sum of irreducible representations

$$P^{3,0} = \Gamma_1' \oplus \Gamma_3 \oplus \Gamma_3', \tag{17}$$

where the representations on the right-hand side occur on the polynomials

$$\Gamma_1': \quad xyz,$$

$$\Gamma_3: \quad \{*x(y^2 - z^2)\},$$

$$\Gamma_3': \quad \{*x(2x^2 - 3y^2 - 3z^2)\} = \{*x(5x^2 - 2r^2)\}. \tag{18}$$

Since this decomposition is less obvious than the simple result for second-rank tensors, we note that the decomposition in Eq. (17) is found using the character table and that vectors in Eq. (18) can be constructed systematically using projection operations [26]. The elementary calculations are not given here. It follows from Eqs. (16) and (17) that

$$P^3 = \Gamma_1' \oplus \Gamma_3 \oplus 2\Gamma_3'. \tag{19}$$

It could be surprising that a cubic polynomial $x(y^2 - z^2)$ appears in a representation Γ_3 corresponding to a second-rank tensor. This circumstance can perhaps be explained by a simple table as follows:

$$\begin{array}{ccc|ccc|ccc} x & y & z & yz & zx & xy & x(y^2-z^2) & y(z^2-x^2) & z(x^2-y^2) \\ -x & z & y & yz & -yx & -xz & x(y^2-z^2) & -z(x^2-y^2) & -y(z^2-x^2) \end{array} \tag{20}$$

The first three columns represent the special symmetry operation $(x,y,z) \to (-x,z,y)$, and the second three columns show the corresponding transformation of the three variables $*(yz)$: since these linear transformations are obviously distinct, this symmetry operation distinguishes between Γ_3 and Γ_3'. The final three columns exhibit the transformation of the quantities $*\{x(y^2 - z^2)\}$: they obviously transform like the variables $*\{yz\}$—that is, by Γ_3 rather than by Γ_3'. In the complete group of 48 symmetries of the cube, these two occurrences of Γ_3 would split into two representations with opposite parity under inversion. This point will be discussed further later in the paper.

[2] See in particular p. 149. From Weyl's standpoint, we are considering the special case of fully symmetric tensors (equivalent to homogeneous polynomials); Weyl's much more general presentation concerns tensors of arbitrary symmetry.

For homogeneous quartic polynomials

$$P^4 = r^4 P^0 \oplus r^2 P^{2,0} \oplus P^{4,0}, \tag{21}$$

and under the group of rotations of the cube, we have the decomposition

$$P^{4,0} = \Gamma_1 \oplus \Gamma_2 \oplus \Gamma_3 \oplus \Gamma_3', \tag{22}$$

where the representations on the right side occur on the polynomials

$$\Gamma_1: \quad \{I_4\},$$

$$\Gamma_2: \quad \{*3(x^4 - 6x^2y^2 + y^4) - 2I_4\},$$

$$\Gamma_3': \quad \{*xy(x^2 - y^2)\},$$

$$\Gamma_3: \quad \{*yz(6x^2 - y^2 - z^2)\}, \tag{23}$$

where $I_4 := (x^4 + y^4 + z^4) - 3(x^2y^2 + y^2z^2 + z^2x^2) = r^4 - 5(x^2y^2 + y^2z^2 + z^2x^2)$.

To summarize, we began with the decompositions given by Eqs. (13), (16), and (21) of the homogeneous polynomials P^2, P^3, and P^4 of degrees 2, 3, and 4 into multiples of powers of invariant r^2 and the remaining polynomials $P^{2,0}$, $P^{3,0}$, and $P^{4,0}$, which are not multiples of powers of r^2. The representations of SO(3) on the vector spaces $P^{2,0}$, $P^{3,0}$, and $P^{4,0}$ are well known to be irreducible [29], but the representations of the group of rotations of the cube on these spaces are reducible and their decompositions into irreducible representations are given as Eqs. (14), (17), and (22) in terms of the explicit polynomial sets defined in Eqs. (7), (18), and (23). The reducibility of these representations is closely linked to the possibility of incomplete tensors; this connection will be developed in the next section.

III. MATRIX A: CONSTRUCTION OF MODELS

In Sec. II A, a basis $\{\tilde{c}_i\}$ of the linear span of the finite set C is constructed in which the basis elements transform by irreducible representations of the group of rotations of the cube; the corresponding basis of polynomials $\{\tilde{p}_j\}$ is constructed in Sec. II B. The velocities and polynomials are now combined by evaluating the matrix A using these bases; the result will be denoted by $\tilde{\mathsf{A}}$. Recall that entries of $\tilde{\mathsf{A}}$ vanish whenever $\tilde{\boldsymbol{c}}_i$ and $\tilde{\boldsymbol{p}}_j$ transform by different irreducible representations so that $\tilde{\mathsf{A}}$ has a block structure which makes it easier to analyze than the original matrix A.

The orthogonality properties of irreducible representations imply another simple but useful conclusion: assume that the set of velocities C has been chosen and that the representation of the group of rotations of a cube on the linear span of C admits the decomposition into irreducible representations

$$\mathsf{C} = n_1\Gamma_1 \oplus n_1'\Gamma_1' \oplus n_2\Gamma_2 \oplus n_3\Gamma_3 \oplus n_3'\Gamma_3'. \tag{24}$$

In order that A have full rank, it is necessary that the representation of the linear span on the polynomial set P admit exactly the same decomposition

$$\mathsf{P} = n_1\Gamma_1 \oplus n_1'\Gamma_1' \oplus n_2\Gamma_2 \oplus n_3\Gamma_3 \oplus n_3'\Gamma_3'. \tag{25}$$

Equations (24) and (25) provide a useful *a priori* constraint on the polynomial set given the discrete velocity set. These equations significantly refine the obvious condition that the velocity and polynomial sets must have the same dimension

$$\dim \mathsf{C} = \dim \mathsf{P} \tag{26}$$

by identifying this common dimension as $\dim \mathsf{C} = \dim \mathsf{P} = n_1 + n_1' + 2n_2 + 3n_3 + 3n_3'$ and by stating that the individual multiplicities n_1, n_1', n_2, n_3, and n_3' must be equal.

The conditions (24) and (25) are only necessary, because nothing prevents the rank of these blocks $\langle \tilde{\boldsymbol{p}}_i | \tilde{\boldsymbol{c}}_i \rangle$ from having less than maximal rank, which must also be checked. Obviously, however, checking the rank of these blocks is much simpler than checking the rank of the entire matrix A. The process is best explained by examples.

A. D3Q6 model

The simplest discrete model is Broadwell's original model with six velocities [30] based on the faces of a cube. Given the velocity set F from Eq. (8), the problem is to choose polynomials to generate appropriate moments. A systematic procedure to guide this choice can be exhibited in tabular form as follows:

	Γ_1	Γ_1'	Γ_2	Γ_3	Γ_3'
D3Q6	1	0	1	0	1
P^0	1	0	0	0	0
P^1	0	0	0	0	1
$P^{2,0}$	0	0	1	1	0

(27)

The first row, labeled "D3Q6," shows the multiplicities of the irreducible representations in the decomposition of the representation of the group of rotations of the cube on the linear span of the discrete velocity set, in this case the set F. The decompositions of the representations on polynomials of degrees 0, 1, and 2 are given in the next lines. It is understood that P^0 can be any scalar r^{2n}—that is, any polynomial set that transforms like $\{1\}$—and P^1 can be any set $r^{2n}\{*x\}$—that is, any polynomial set that transforms like $\{*x\}$. If they are linearly independent, the moments defined by each row are components of a complete tensor: in this case, the second row can define a scalar, the third row a vector, and the last row a trace-free second-rank tensor. The goal is to choose entire rows as nearly as possible to construct the model.

Comparison of the first row with the others shows immediately that the model must contain contributions from each row: for example, to obtain the representation Γ_1, we must include P^0, and to obtain Γ_3', we must include P_1; however, the trial set $P^0 \oplus P^1 \oplus P^{2,0}$, corresponding to a scalar, a vector, and a trace-free second-rank tensor, has dimension 9. Since its dimension exceeds the number of discrete velocities, the moments generated by these polynomials cannot be linearly independent. The explanation is that, as noted earlier, the quadratic polynomials that transform as Γ_3, $*\{xy\}$ vanish identically on the set F. We cannot include all of the polynomials in $P^{2,0}$ to form the model, but are forced instead to select only the occurrence of Γ_2. The model based on D3Q6 therefore necessarily contains an incomplete second-rank tensor.[3]

The set of polynomials corresponding to the velocity set F must be

$$\Gamma_1 \quad \text{from} \quad P^0{:}\{1\},$$

$$\Gamma_3' \quad \text{from} \quad P^1{:}\{*x\},$$

$$\Gamma_2 \quad \text{from} \quad P^{2,0}{:}\{*(x^2 - y^2)\}. \tag{28}$$

It remains to verify that the polynomials actually are linearly independent over the discrete velocity set. In this case, the verification amounts to showing that no polynomial set vanishes identically on the set of points that transforms by the same irreducible representation. The trivial verification is omitted.

B. D3Q15 model

The table corresponding to Eq. (27) is

	Γ_1	Γ_1'	Γ_2	Γ_3	Γ_3'
D3Q15	3	1	1	1	2
P^0	1	0	0	0	0
P^1	0	0	0	0	1
$P^{2,0}$	0	0	1	1	0
$P^{3,0}$	0	1	0	1	1

(29)

$P^{3,0}$ must be included in order to accommodate the occurrence of Γ_1' in D3Q15. However, the table immediately shows that the moments formed from $P^{3,0}$ cannot be the components of a complete third-rank tensor, because $P^{3,0}$ and $P^{2,0}$ generate two occurrences of Γ_3, while D3Q15 can only have one. A suitable polynomial set is

$$3\Gamma_1{:} \quad \{1\},\{r^2\},\{r^4\},$$

$$2\Gamma_3'{:} \quad \{*x\},\{*xr^2\},$$

$$\Gamma_2{:} \quad \{*(x^2 - y^2)\},$$

$$\Gamma_3{:} \quad \{*xy\},$$

$$\Gamma_1'{:} \quad \{xyz\}. \tag{30}$$

The table of representations again suggests the degeneracies that must occur in this model. We have seen that the set $P^{3.0}$ generates a redundant occurrence of Γ_3, and indeed, the cubics that transform as Γ_3, given in Eq. (18) as $\{*x(y^2 - z^2)\}$, all vanish identically on the velocity set D3Q15. The remaining cubics $*x(2x^2 - 3y^2 - 3z^2)$, which transform as Γ_3', prove to be linearly dependent on the polynomials selected in Eq. (30), but we omit the simple verification.

[3]It should be noted that this fact was irrelevant to Broadwell's work.

We must again verify that these polynomials are linearly independent over the discrete set of velocities $\mathsf{F}\cup\mathsf{V}\cup\mathsf{O}$ that defines this model. For the irreducible representations that only occur once, it is sufficient to verify that the polynomials do not vanish identically. In this case, these representations are Γ_2 and Γ_3, corresponding to quadratic polynomials. We omit the easy verification. A nontrivial problem arises only for the irreducible representations that occur with multiplicity greater than one. Let us verify directly that the three polynomials that transform according to Γ_1 are linearly independent in this model. Using the results of the Appendix, the identity representation occurs on $\Sigma_{\boldsymbol{c}_i\in\mathsf{O}}\boldsymbol{c}_i$, $\frac{1}{6}\Sigma_{\boldsymbol{c}_i\in\mathsf{F}}\boldsymbol{c}_i$, and $\frac{1}{8}\Sigma_{\boldsymbol{c}_i\in\mathsf{V}}\boldsymbol{c}_i$. Evaluating the polynomials 1, r^2, and r^4 on these three functions gives the matrix

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 3 & 9 \end{bmatrix}. \tag{31}$$

Since this matrix is nonsingular, the required linear independence is demonstrated. A similar argument applies to the two occurrences of the representation Γ_3' and establishes that the polynomials in Eq. (30) are indeed linearly independent over the velocity set D3Q15.

In the notation of Eq. (4), the distribution function of this model is the finite sum

$$f(\boldsymbol{x},\boldsymbol{c},t)=\sum_{\boldsymbol{c}_i\in\mathsf{F}\cup\mathsf{V}\cup\mathsf{O}} f_i(\boldsymbol{x},t)\hat{\boldsymbol{c}}_i. \tag{32}$$

We have verified that the following linearly independent moments are possible in this model:

$$\rho=\langle 1|f\rangle, \tag{33a}$$

$$e=\langle r^2|f\rangle, \tag{33b}$$

$$\varepsilon=\langle r^4|f\rangle, \tag{33c}$$

$$\boldsymbol{j}=\langle * x|f\rangle, \tag{33d}$$

$$\boldsymbol{q}=\langle * xr^2|f\rangle, \tag{33e}$$

$$\mathsf{p}=\langle *(x^2-y^2), * xy|f\rangle, \tag{33f}$$

$$\mathsf{T}=\langle xyz|f\rangle, \tag{33g}$$

where the left-hand side denotes a tensor with components given by the moments on the right-hand side. The scalars in this model are the mass density ρ, a quantity e formally related to the internal energy, and a fourth-order moment ε. The vectors in this model are the momentum $\boldsymbol{j}$ and the vector $\boldsymbol{q}$ related to the energy flux. One trace-free second-rank tensor exists, the momentum flux, or stress p. All of these tensors are complete. T is an incomplete third-rank tensor.

We recall that the analysis is restricted to the kinematics of moments. By stating that the model contains a vector formally related to an energy flux, we only assert that $\mathbf{q}$ is a contracted third-rank tensor that transforms properly as a vector; we do not assert that the D3Q15 model correctly models the heat flux.

C. D3Q13 and D3Q19 models

Without presenting the straightforward details, we denote the moments in the D3Q13 model,

$$\rho=\langle 1|f\rangle, \tag{34a}$$

$$e=\langle r^2|f\rangle, \tag{34b}$$

$$\boldsymbol{j}=\langle * x|f\rangle, \tag{34c}$$

$$\mathsf{p}=\langle *(x^2-y^2), * xy|f\rangle, \tag{34d}$$

$$\mathsf{T}=\langle * x(y^2-z^2)|f\rangle, \tag{34e}$$

where the distribution function is

$$f(\boldsymbol{x},\boldsymbol{c},t)=\sum_{\boldsymbol{c}_i\in\mathsf{E}\cup\mathsf{O}} f_i(\boldsymbol{x},t)\hat{\boldsymbol{c}}_i. \tag{35}$$

The moment T is an incomplete third-rank tensor.

For the D3Q19 model, the moments are

$$\rho=\langle 1|f\rangle, \tag{36a}$$

$$e=\langle r^2|f\rangle, \tag{36b}$$

$$\varepsilon=\langle r^4|f\rangle, \tag{36c}$$

$$\boldsymbol{j}=\langle * x|f\rangle, \tag{36d}$$

$$\boldsymbol{q}=\langle * xr^2|f\rangle, \tag{36e}$$

$$\mathsf{p}=\langle *(x^2-y^2), * xy|f\rangle, \tag{36f}$$

$$\mathsf{e}=\langle *(x^2-y^2)r^2, * xyr^2|f\rangle, \tag{36g}$$

where the distribution function is

$$f(\boldsymbol{x},\boldsymbol{c},t)=\sum_{\boldsymbol{c}_i\in\mathsf{F}\cup\mathsf{E}\cup\mathsf{O}} f_i(\boldsymbol{x},t)\hat{\boldsymbol{c}}_i. \tag{37}$$

In this model, the flux of $\boldsymbol{q}$ is defined by the trace-free second-rank tensor e and the scalar e. Whereas the D3Q13 and D3Q15 models both contain incomplete tensors, all moments in the D3Q19 model are complete. This model is observed to be numerically more stable than the D3Q15 model [31].

D. D3Q27 model

We will not repeat the previous tabular procedure for choosing the polynomials: we merely recall from Eq. (11) that the points of the D3Q27 model decompose into $4\Gamma_1 \oplus \Gamma_1' \oplus 2\Gamma_2 \oplus 3\Gamma_3 \oplus 3\Gamma_3'$. Consider the candidate polynomials

$$4\Gamma_1: \quad \{1\},\{r^2\},\{r^4\},\{r^6\},$$

$$\Gamma_1': \quad \{xyz\},$$

$$2\Gamma_2: \quad \{*(x^2-y^2)\},\{*(x^2-y^2)r^2\},$$

$$3\Gamma_3: \quad \{*xy\},\{*xyr^2\},\{*x(y^2-z^2)\},$$

$$3\Gamma_3': \quad \{*x\},\{*xr^2\},\{*x(2x^2-3y^2-3z^2)\}. \tag{38}$$

In this case, the moments generated by the indicated polynomial sets are not linearly independent over the velocity set chosen. The linear dependence proves to occur in the three occurrences of Γ_3'. As in the analysis of the D3Q15 model, we must evaluate the nine polynomials $\{*x\}$, $\{*xr^2\}$, and $\{*x(2x^2-3y^2-3z^2)\}$ on the nine functions

$$\tilde{\boldsymbol{c}}_\alpha = \frac{1}{6}\sum_{\boldsymbol{c}_i\in \mathsf{F}} c_{i\alpha}\hat{\boldsymbol{c}}_i, \quad \tilde{\boldsymbol{c}}'_\alpha = \frac{1}{8}\sum_{\boldsymbol{c}_i\in \mathsf{V}} c_{i\alpha}\hat{\boldsymbol{c}}_i, \quad \tilde{\boldsymbol{c}}''_\alpha = \frac{1}{8}\sum_{\boldsymbol{c}_i\in \mathsf{E}} c_{i\alpha}\hat{\boldsymbol{c}}_i,$$

$$\alpha = 1,2,3,$$

in which Γ_3' occurs. We simply state the result of the calculation:

$$\begin{bmatrix} \langle x_\beta|\hat{\tilde{c}}_\alpha\rangle & \langle r^2x_\beta|\hat{\tilde{c}}_\alpha\rangle & \langle x_\beta(2x_\beta^2-3x_{\beta+1}^2-3x_{\beta+2}^2)|\hat{\tilde{c}}_\alpha\rangle \\ \langle x_\beta|\hat{\tilde{c}}'_\alpha\rangle & \langle r^2x_\beta|\hat{\tilde{c}}'_\alpha\rangle & \langle x_\beta(2x_\beta^2-3x_{\beta+1}^2-3x_{\beta+2}^2)|\hat{\tilde{c}}'_\alpha\rangle \\ \langle x_\beta|\hat{\tilde{c}}''_\alpha\rangle & \langle r^2x_\beta|\hat{\tilde{c}}''_\alpha\rangle & \langle x_\beta(2x_\beta^2-3c_{i\beta+1}^2-3c_{i\beta+2}^2)|\hat{\tilde{c}}''_\alpha\rangle \end{bmatrix} = \begin{bmatrix} 2\mathsf{I}_{3\times3} & 2\mathsf{I}_{3\times3} & 4\mathsf{I}_{3\times3} \\ 8\mathsf{I}_{3\times3} & 24\mathsf{I}_{3\times3} & -32\mathsf{I}_{3\times3} \\ 8\mathsf{I}_{3\times3} & 16\mathsf{I}_{3\times3} & -8\mathsf{I}_{3\times3} \end{bmatrix}. \tag{39}$$

Since

$$\det\begin{bmatrix} 2 & 2 & 4 \\ 8 & 24 & -32 \\ 8 & 16 & -8 \end{bmatrix} = 0, \tag{40}$$

we see that the three polynomials which transform as Γ_3' are not linearly independent of the set of velocities chosen.

Lallemand *et al.* [8] observed that the linear independence could be restored by replacing the velocities corresponding to the faces by the vectors $\mathsf{F}^* = \{(\pm 2,0,0),(0,\pm 2,0),(0,0,\pm 2)\}$. This alteration does not change any of the decompositions into irreducible representations; however, routine calculation shows that the polynomials which transform as Γ_3' are linearly independent over the set $\mathsf{F}^*\cup\mathsf{E}\cup\mathsf{V}\cup\mathsf{O}$ and that the following moments are linearly independent:

$$\rho = \langle 1|f\rangle, \tag{41a}$$

$$e = \langle r^2|f\rangle, \tag{41b}$$

$$\varepsilon_1 = \langle r^4|f\rangle, \tag{41c}$$

$$\varepsilon_2 = \langle r^6|f\rangle, \tag{41d}$$

$$\boldsymbol{j} = \langle *x|f\rangle, \tag{41e}$$

$$\boldsymbol{q} = \langle *xr^2|f\rangle, \tag{41f}$$

$$\mathsf{p} = \langle *(x^2-y^2), *xy|f\rangle, \tag{41g}$$

$$\mathsf{e} = \langle *(x^2-y^2)r^2, *xyr^2|f\rangle, \tag{41h}$$

$$\mathsf{T} = \langle xyz, *x(y^2-z^2), *x(2x^2-3y^2-3z^2)|f\rangle, \tag{41i}$$

where the distribution function is

$$f(\boldsymbol{x},\boldsymbol{c},t) = \sum_{\boldsymbol{c}_i\in\mathsf{F}^*\cup\mathsf{E}\cup\mathsf{V}\cup\mathsf{O}} f_i(\boldsymbol{x},t)\hat{\boldsymbol{c}}_i. \tag{42}$$

In this model, a fourth scalar ε_2 exists and the third-rank tensor T is complete. Equations (21) and (22) show that the set of all quartics decomposes into irreducible representations as $P^4 = 4\Gamma_1\oplus\Gamma_1'\oplus 3\Gamma_2\oplus 4\Gamma_3\oplus 4\Gamma_3'$ and contains more occurrences of Γ_3 and Γ_3' than admitted by the velocity set. Correspondingly, we observe that the three quartic polynomials $*xy(x^2-y^2)$ that transform as Γ_3' [compare Eq. (23)] vanish on the velocity set.

IV. HIGHER-ORDER MODEL: D3Q51

We next consider a higher-order model. Since the quartics $*xy(x^2-y^2)$ vanish on the discrete velocity sets based on the edges, vertices, faces, and center of a cube, in any model based on these sets of vectors or on sets of their scalar multiples, fourth-rank tensors cannot be complete. For example, adding the 6 velocities $\{(\pm 3,0,0),(0,\pm 3,0),(0,0,\pm 3)\}$ or the 12 velocities $\{(0,\pm 2,\pm 2),(\pm 2,0,\pm 2),(\pm 2,\pm 2,0)\}$ to the D3Q27 model will result in more complexity, but not in complete fourth-rank tensors. To obtain them, a different kind of velocity set must be added.

A general vector has 24 distinct images under the 24 rotations of the cube; the edges, faces, and vertices have fewer because they are invariant under special rotations. To find a velocity set on which the quartics $*xy(x^2-y^2)$ do not vanish identically, it is necessary to add 24 velocities found as the distinct images of a single vector under the group of rotations of the cube: a model in which tensors of rank 4 can be complete must contain at least 51 velocities.

One alternative is to add the 24 velocities obtained as the images of the vector (2,1,0). This set contains the velocities with the smallest energy beyond the D3Q27 model; it is denoted as

$$\mathsf{G} = \{(\pm 2,\pm 1,0),(\pm 1,\pm 2,0),(\pm 2,0,\pm 1),(\pm 1,0,\pm 2), (0,\pm 2,\pm 1),(0,\pm 1,\pm 2)\}. \tag{43}$$

The representation of the group of rotations of the cube on the linear span of this set decomposes into the irreducible representations

$$\mathsf{G} = \Gamma_1\oplus\Gamma_1'\oplus 2\Gamma_2\oplus 3\Gamma_3\oplus 3\Gamma_3'. \tag{44}$$

The representation of the group of rotations of the cube on the linear span of any set of 24 points obtained as the distinct images of one lattice point will always admit the same decomposition into irreducible representations as Eq. (44): this is the "regular representation" of group theory. We add that any set of vectors, obtained from any single vector by the operations of the group of rotations of the cube, must contain either 1, 6, 8, 12, or 24 distinct vectors and must define a representation which decomposes into irreducible representations like one of the sets O, F, V, E, or G; there are no other possibilities.

Let us consider the discrete velocity set of the D3Q27 model augmented by the set G, giving the velocity set D3Q51 $=\mathsf{O}\cup\mathsf{F}^*\cup\mathsf{V}\cup\mathsf{E}\cup\mathsf{G}$. The representation of the group of rotations of the cube on the linear span of this set decomposes into irreducible representations as

$$\mathsf{O}\oplus\mathsf{F}^*\oplus\mathsf{V}\oplus\mathsf{E}\oplus\mathsf{G}=5\Gamma_1\oplus 2\Gamma_1'\oplus 4\Gamma_2\oplus 6\Gamma_3\oplus 6\Gamma_3'. \tag{45}$$

We again exhibit the choice of polynomials in tabular form:

	Γ_1	Γ_1'	Γ_2	Γ_3	Γ_3'
D3Q51	5	2	4	6	6
P^0	1	0	0	0	0
P^1	0	0	0	0	1
$P^{2,0}$	0	0	1	1	0
$P^{3,0}$	0	1	0	1	1
$P^{4,0}$	1	0	1	1	1
$P^{5,0}$	0	0	1	1	2
$P^{6,0}$	1	1	1	2	1

(46)

The first line shows that this model requires two polynomials that transform as Γ_1'. Finding these polynomials proves to be nontrivial. The obvious choice xyz and r^2xyz is unsatisfactory because both vanish on the sets G, F, and E and they coincide on V. It follows that xyz and r^2xyz are not linearly independent of D3Q51. The problem can be solved by introducing polynomials of degree 6 since Γ_1' occurs on the polynomial

$$p_6(x,y,z)=x^2y^2(x^2-y^2)+y^2z^2(y^2-z^2)+z^2x^2(z^2-x^2), \tag{47}$$

which obviously does not vanish on the set G. This polynomial and xyz give two linearly independent polynomials that transform by Γ_1'.

Using this choice, we find that the choice of polynomials

$$5\Gamma_1:\quad \{1\},\{r^2\},\{r^4\},\{r^6\},\{x^4+y^4+z^4-3(x^2y^2+y^2z^2+z^2x^2)\},$$

$$2\Gamma_1':\quad \{xyz\},\{x^2y^2(x^2-y^2)+y^2z^2(y^2-z^2)+z^2x^2(z^2-x^2)\},$$

$$4\Gamma_2:\quad \{*(x^2-y^2)\},\{*(x^2-y^2)r^2\},\{*(x^2-y^2)r^4\},$$
$$\{*(x^4+y^4-2z^4-12x^2y^2+6y^2z^2+6z^2x^2)\},$$

$$6\Gamma_3:\quad \{*xy\},\{*xyr^2\},\{*xyr^4\},\{*x(y^2-z^2)\},$$
$$\{*x(y^2-z^2)r^2\},\{*yx(6x^2-y^2-z^2)\},$$

$$6\Gamma_3':\quad \{*x\},\{*xr^2\},\{*x(2x^2-3y^2-3z^2)\},\{*xy(x^2-y^2)\},$$
$$\{*(x^4z-6x^2y^2z+y^4z)\},\{*(2x^5-10x^3(y^2+z^2)+5x(y^4+z^4))\} \tag{48}$$

yields a D3Q51 model in which the tensors in Eq. (39) are all complete and in which the following additional tensor of rank 4 is also complete:

$$\begin{aligned}\mathsf{S}=\langle & x^4+y^4+z^4-3(x^2y^2+y^2z^2+z^2x^2),\\ & *(x^4+y^4-2z^4-12x^2y^2+6y^2z^2+6z^2x^2),\ *xy(x^2-y^2),\\ & *(6x^2yz-y^3z-yz^3)|f\rangle\ .\end{aligned} \tag{49}$$

The model contains incomplete tensors of ranks 5 and 6.

In this case, the vanishing of the polynomial xyz on the set G caused difficulties. An alternative is to add points on which xyz does not vanish—for example, the images of the velocity vector (3,2,1). Although this possibility will not be pursued here, we note that since there are only 24 images of this point under the group of rotations of the cube, to obtain the set of 48 points of the form $\Pi(\pm 3,\pm 2,\pm 1)$, where Π indicates the six permutations of (3,2,1), it would be necessary to add the 24 images of the point $(-3,-2,-1)$. This suggests the question whether it would not be more natural to use the complete group of 48 symmetries of the cube, including inversions; this question will be addressed in Sec. VI.

This example illustrates some of the difficulties in constructing higher-order models: tensors of rank 4 are incomplete in D3Q27 because of the vanishing of three quartics; in order to achieve complete quartics, 24 velocities were added to the model, yet tensors of rank 5 remain incomplete.

V. TWO-DIMENSIONAL MODELS

To treat two-dimensional models by the group-theoretic approach, the rotation group of the cube is replaced by a symmetry group of the square. It will be taken to be a group of eight transformations: the four 90° rotations and the four reflections through the diagonals and the bisectors of opposite sides. This group is larger than the group of four rotations of the square and is chosen to provide as many representations as possible. The choice of the symmetry group will be discussed further in the next section.

The irreducible representations are

Repr.	Polynomials
Γ_1	1
Γ_2	x,y
Γ_1'	(x^2-y^2)
Γ_1''	xy
Γ_1'''	$xy(x^2-y^2)$

(50)

The simplest sets of discrete velocities invariant under this symmetry group are formed from the faces and vertices of the square, to which we add as before the center,

$$\mathsf{F}=\{(1,0),(0,1),(-1,0),(0,-1)\},$$

$$\mathsf{V}=\{(1,1),(-1,1),(-1,-1),(1,-1)\},$$

$$\mathsf{O} = \{(0,0)\}.$$

The corresponding representations decompose into irreducible representations as

$$\mathsf{F} = \Gamma_1 \oplus \Gamma_2 \oplus \Gamma_1',$$

$$\mathsf{V} = \Gamma_1 \oplus \Gamma_2 \oplus \Gamma_1'',$$

$$\mathsf{O} = \Gamma_1.$$

As in the symmetry group of the cube, the representation of the continuous rotation group on trace-free second-rank tensors, given as the representation on quadratics $\{(x^2-y^2), 2xy\}$, splits into $\Gamma_1' \oplus \Gamma_1''$. To describe a second-rank tensor completely, both representations are needed.

The simplest model in which a second-rank tensor is complete D2Q9, defined by the set $\mathsf{F} \cup \mathsf{V} \cup \mathsf{O}$. Since the representation on these velocities decomposes into

$$\mathsf{F} \oplus \mathsf{V} \oplus \mathsf{O} = 3\Gamma_1 \oplus 2\Gamma_2 \oplus \Gamma_1' \oplus \Gamma_1'', \tag{51}$$

we choose candidate polynomials belonging to the same representations,

$$3\Gamma_1: \quad \{1\},\{r^2\},\{r^4\},$$

$$2\Gamma_2: \quad \{x,y\},\{xr^2,yr^2\},$$

$$\Gamma_1': \quad x^2 - y^2,$$

$$\Gamma_1'': \quad xy.$$

These moments are easily shown to be linearly independent over the defining velocity set; accordingly, this nine-velocity model describes the following moments:

$$\rho = \langle 1|f\rangle, \tag{52a}$$

$$e = \langle r^2|f\rangle, \tag{52b}$$

$$\varepsilon_1 = \langle r^4|f\rangle, \tag{52c}$$

$$\boldsymbol{j} = \langle x,y|f\rangle, \tag{52d}$$

$$\boldsymbol{q} = \langle r^2x, r^2y|f\rangle, \tag{52e}$$

$$\mathsf{p} = \langle x^2y^2, xy|f\rangle. \tag{52f}$$

To obtain a complete third-rank tensor, we can add the velocities $\mathsf{F}^* = \{(2,0),(0,2),(-2,0),(0,-2)\}$, resulting in a model D2Q13. The representation on the velocity set $\mathsf{F} \cup \mathsf{F}^* \cup \mathsf{V} \cup \mathsf{O}$ decomposes into

$$\mathsf{F} \oplus 2\mathsf{F} \oplus \mathsf{V} \oplus \mathsf{O} = 4\Gamma_1 \oplus 3\Gamma_2 \oplus 2\Gamma_1' \oplus \Gamma_1''. \tag{53}$$

The polynomial set

$$4\Gamma_1: \quad \{1\},\{r^2\},\{r^4\},\{r^6\},$$

$$3\Gamma_2: \quad \{x,y\},\{xr^2,yr^2\},\{x(x^2-3y^2),y(3x^2-y^2)\},$$

$$2\Gamma_1': \quad (x^2-y^2),(x^2-y^2)r^2,$$

$$\Gamma_1'': \quad xy$$

is easily shown to be linearly independent over the chosen finite velocity space.

Let us briefly consider the formulation of higher-order models. Eight more velocities can be added to F, V, and O, either as the set $\mathsf{F}^* \cup \mathsf{V}^* = \{\pm 2,0),(0,\pm 2),(\pm 2,\pm 2)\}$ or, following the D3Q51 model, as the set $\mathsf{G} = \{(\pm 2,\pm 1),(\pm 1,\pm 2)\}$. The first set leads to a 17-velocity model in two dimensions, which like D2Q9 cannot describe a complete fourth-rank tensor: the polynomial $xy(x^2-y^2)$ still vanishes on all of the discrete velocities. On the other hand, the representation on G decomposes as $\mathsf{G} = \Gamma_1 \oplus \Gamma_1' \oplus \Gamma_1'' \oplus \Gamma_1''' \oplus 2\Gamma_2$. The resulting D2Q17 model contains a complete fourth-rank tensor.

VI. CHOICE OF THE SYMMETRY GROUP

In this paper, the symmetry group of the velocity set is introduced only in order to facilitate counting the linearly independent moments by exploiting the orthogonality properties of distinct irreducible representations; no special physical importance is attached to the symmetry group. Thus, the group of rotations of a cube was chosen simply for ease of exposition. It might seem equally natural to choose the group of 48 symmetries that includes the inversions $(x,y,z) \to (-x,-y,-z)$ instead. The representation theory of this group yields two irreducible representations with opposite parity under inversions for every irreducible representation of the group of 24 rotations. This distinction can be between representations on polynomials of even and odd order. Examples encountered in this paper include the representation of Γ_1' on the polynomials xyz and $x^2y^2(x^2-y^2)+y^2z^2(y^2-z^2)+z^2x^2(z^2-x^2)$ where the first changes sign under inversions while the second is invariant, and the representations of Γ_3 on $*\{xy\}$ and on $*\{x(y^2-z^2)\}$, where the first is invariant under inversions while the second changes sign. In both cases, the two representations of the complete group of 48 symmetries of the cube are inequivalent, but the representations of the group of 24 rotations of the cube are equivalent.

For the purposes of this paper, then, little would be gained by introducing the group of 48 symmetries of the cube instead of the group of 24 rotations: the result would simply be an irrelevant distinction between odd- and even-order polynomials. However, if a theory that distinguishes between axial and polar quantities is required, then the representation theory of the complete group of 48 symmetries of the cube would indeed be relevant for physical reasons. The two-relaxation-time (TRT) LBE models [32,33] are examples in which the moment basis is decomposed into its symmetric and antisymmetric parts.

The choice of symmetry group in the two-dimensional case raises a different issue. If we had made the obvious choice of the group of four rotations of a square, there would only be four irreducible representations. By choosing a larger group with more irreducible representations, we can increase the number of vanishing elements in the matrix A, thereby lightening the algebra.

VII. CONCLUSIONS

The representation theory of finite groups has been applied to the systematic construction of lattice Boltzmann models in the moment-based formulation of d'Humières *et al.* [5,13,27]. Given the choice of a finite velocity set $\{\boldsymbol{c}_i\}$, the method helps identify the tensors for which a kinematically satisfactory description is possible: here, "kinematically satisfactory" simply means that the tensor in the discrete theory has the same number of linearly independent components as its continuous counterpart. Although these tensors can be identified by elementary means, group theory introduces natural vector space bases in which the calculations are particularly simple.

To illustrate the utility of group representation theory, we cite the simple necessary condition for completeness of tensors given by Eqs. (24) and (25) that generalizes the obvious dimension count, Eq. (26). Once the velocity set is chosen, this condition significantly restricts the types of tensors that can be complete in the model.

As a second example, we cite the introduction of the point set $\{(\pm 2,\pm 1,0),(\pm 1,\pm 2,0),(\pm 2,0,\pm 1),(\pm 1,0,\pm 2),(0,\pm 2,\pm 1),(0,\pm 1,\pm 2)\}$ to the D3Q27 model in order to obtain complete fourth-rank tensors: without group theory, it might not be obvious that the addition of point sets based on scalar multiples of the edges, faces, and vertices will not lead to the desired result.

As a final example, we cite the introduction of sixth-order polynomials in the construction of the model D3Q51 in order to obtain a second instance of the representation Γ_1'. Trial and error would also lead to this conclusion, but it is reasonable to say that group theory provides a simple explanation: sextic, but not quintic, polynomials furnish a linearly independent occurrence of Γ_1'.

By increasing the dimension of the space of moments, adding more velocities makes complete tensors of higher rank possible. Thus, in three dimensions, the Broadwell model based on six velocities contains an incomplete second-rank tensor; in the D3Q15 and D3Q19 models, the second-rank tensors are complete, but a third-rank tensor is incomplete; in the D3Q27 model, the lowest rank of an incomplete tensor is 4. A similar progression occurred for the two-dimensional models.

We would like to comment on some applications of models in which tensors of high rank are complete. The analysis of Lallemand and co-workers [5,8,9] requires computing the dispersion relation of waves of finite wave number in order to assess the numerical stability of the method. From this viewpoint, the present analysis is restricted to the zero-wave-number limit. The wave dispersion relations couple the higher-order moments, the completeness properties of which will then have a role in the finite-wave-number properties of the model.

Another possible application is to extended thermodynamics [34,35], where dynamic equations for nonconserved moments like the stress and heat flux are derived. The Grad 13-velocity model is the starting point for such modeling. By providing complete moments up to order 4, models like D3Q51 can be the basis of a discrete extended thermodynamics. Although further research will be necessary to determine the applicability of such models, it is evident that they exhibit the minimal complexity needed to advance beyond Navier-Stokes hydrodynamics in the discrete setting.

APPENDIX: SYMMETRY GROUP OF THE CUBE

This appendix lists the decompositions into irreducible representations of the representations of the symmetry group of the cube on the faces, edges, and vertices.

Denote the vectors corresponding to the faces of the cube as $\boldsymbol{c}_1=(1,0,0)$, $\boldsymbol{c}_2=(-1,0,0)$, $\boldsymbol{c}_3=(0,1,0)$, $\boldsymbol{c}_4=(0,-1,0)$, $\boldsymbol{c}_5=(0,0,1)$, and $\boldsymbol{c}_6=(0,0,-1)$. The decomposition of the functions on these vectors into irreducible representations is given by the linear combinations

F	$\boldsymbol{c}_1$	$\boldsymbol{c}_2$	$\boldsymbol{c}_3$	$\boldsymbol{c}_4$	$\boldsymbol{c}_5$	$\boldsymbol{c}_6$
Γ_1	1	1	1	1	1	1
	1	1	−1	−1	0	0
Γ_2	0	0	1	1	−1	−1
	−1	−1	0	0	1	1
	1	−1	0	0	0	0
Γ_3'	0	0	1	−1	0	0
	0	0	0	0	−1	1

(A1)

The entry corresponding to Γ_3' means that the three linear combinations $(\boldsymbol{c}_1-\boldsymbol{c}_2)$, $(\boldsymbol{c}_3-\boldsymbol{c}_4)$, and $(\boldsymbol{c}_5-\boldsymbol{c}_6)$ transform like a vector under the symmetry group of the cube. Note that the three linear combinations listed as transforming as Γ_2 are linearly dependent.

The linear combinations are of the form $\Sigma_{1\le i\le 6} p_j(\boldsymbol{c}_i)\boldsymbol{c}_i$, where the p_j are polynomials transforming irreducibly as Γ_1, Γ_2, and Γ_3. In Eq. (A1), these polynomials are, respectively, $\{1\}$, $\{*(x^2-y^2)\}$, and $\{*x\}$.

Next, write the vectors corresponding to the eight vertices as $\boldsymbol{c}_1=(1,1,1)$, $\boldsymbol{c}_2=(1,1,-1)$, $\boldsymbol{c}_3=(1,-1,1)$, $\boldsymbol{c}_4=(-1,1,1)$, $\boldsymbol{c}_5=(1,-1,-1)$, $\boldsymbol{c}_6=(-1,1,-1)$, $\boldsymbol{c}_7=(-1,-1,1)$, and $\boldsymbol{c}_8=(-1,-1,-1)$. The decomposition of functions on this set into irreducible representations is given by the linear combinations

V	$\boldsymbol{c}_1$	$\boldsymbol{c}_2$	$\boldsymbol{c}_3$	$\boldsymbol{c}_4$	$\boldsymbol{c}_5$	$\boldsymbol{c}_6$	$\boldsymbol{c}_7$	$\boldsymbol{c}_8$
Γ_1	1	1	1	1	1	1	1	1
Γ_1'	1	1	−1	−1	1	1	1	1
Γ_3	1	1	−1	−1	−1	−1	1	1
	1	−1	−1	1	1	−1	−1	1
	1	−1	1	−1	−1	1	−1	1
Γ_3'	1	1	1	−1	1	−1	−1	−1
	1	1	−1	1	−1	1	−1	−1
	1	−1	1	1	−1	−1	1	−1

(A2)

Finally, denote the vectors corresponding to the edges as $\boldsymbol{c}_1=(1,1,0)$, $\boldsymbol{c}_2=(-1,1,0)$, $\boldsymbol{c}_3=(-1,-1,0)$, $\boldsymbol{c}_4=(1,-1,0)$, $\boldsymbol{c}_5=(0,1,1)$, $\boldsymbol{c}_6=(0,-1,1)$, $\boldsymbol{c}_7=(0,-1,-1)$, $\boldsymbol{c}_8=(0,1,-1)$, $\boldsymbol{c}_9=(1,0,1)$, $\boldsymbol{c}_{10}=(-1,0,1)$, $\boldsymbol{c}_{11}=(-1,0,-1)$, and $\boldsymbol{c}_{12}=(1,0,-1)$. The decomposition of functions on this set into irreducible representations is

$$
\begin{array}{c|cccccccccccc}
\mathsf{E} & \boldsymbol{c}_1 & \boldsymbol{c}_2 & \boldsymbol{c}_3 & \boldsymbol{c}_4 & \boldsymbol{c}_5 & \boldsymbol{c}_6 & \boldsymbol{c}_7 & \boldsymbol{c}_8 & \boldsymbol{c}_9 & \boldsymbol{c}_{10} & \boldsymbol{c}_{11} & \boldsymbol{c}_{12} \\
\hline
\Gamma_1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
\Gamma_2 & 2 & 2 & 2 & 2 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\
 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 & -1 & -1 & -1 & -1 \\
 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\
\Gamma_3' & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\
 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 \\
 & 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 \\
\Gamma_3 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \\
 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\Gamma_3 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 \\
 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1
\end{array}
\tag{A3}
$$

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