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Kinetic theory representation of hydrodynamics: a way beyond the Navier–Stokes equation

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We present in detail a theoretical framework for representing hydrodynamic systems through a systematic discretization of the Boltzmann kinetic equation. The work is an extension of a previously proposed formulation. Conventional lattice Boltzmann models can be shown to be directly derivable from this systematic approach. Furthermore, we provide here a clear and rigorous procedure for obtaining higher-order approximations to the continuum Boltzmann equation. The resulting macroscopic moment equations at each level of the systematic discretization give rise to the Navier–Stokes hydrodynamics and those beyond. In addition, theoretical indications to the order of accuracy requirements are given for each discrete approximation, for thermohydrodynamic systems, and for fluid systems involving long-range interactions. All these are important for complex and micro-scale flows and are missing in the conventional Navier–Stokes order descriptions. The resulting discrete Boltzmann models are based on a kinetic representation of the fluid dynamics, hence the drawbacks in conventional higher-order hydrodynamic formulations can be avoided.

1. Introduction

The fundamental task of non-equilibrium statistical mechanics is to deduce the evolution of the macroscopic state of physical systems from the knowledge of their underlying microscopic dynamics. For a given physical system, descriptions with vastly different degree of detail may be devised depending on the purposes at hand. For the classic gas system consisting of N particles in three-dimensions, the most detailed description is the Hamilton representation which describes the system by the $3N$ generalized coordinates and $3N$ momenta of the consisting particles obeying the Hamilton canonical equation. Alternatively, using the Gibbs ensemble of a large number of identical systems, we can describe the system by a $6N$-dimensional continuum probability distribution function governed by the Liouville equation. This leads exactly to the BBGKY infinite hierarchy, with the kinetic equation governing the evolution of the six-dimensional single-particle distribution function as its first tier (see Bogoliubov 1962; Liboff 1969). If molecular chaos is assumed, the kinetic equation can be closed and the gas system is described by the single-particle distribution function governed by the celebrated Boltzmann equation (see Cercignani 1975). At each level of these reductions, certain details of the previous level of description are deemed as unimportant and sacrificed for greater simplicity and solvability. Obtaining the simplest description that is easy to solve and encompasses as much as possible the essential physics is at the heart of non-equilibrium statistical mechanics. In this paper, we attempt to give a representation of the classical gas systems which includes much of the physics in the kinetic equation yet with a simpler form and better solvability than the conventional thermodynamic descriptions.

Deriving macroscopic descriptions from the kinetic equation was the central topic of kinetic theory during its development. Naturally, as the lowest velocity moments of the distribution function, the thermodynamic variables, i.e. density, flow velocity and temperature, satisfy the conservation equations of mass, momentum and energy. However, the conservation equations are not closed because of the presence of higher moments such as the momentum stress and heat flux. In the conventional Chapman–Enskog successive approximation (Chapman & Cowling 1970), closures are made by approximating the fluxes in terms of the basic state variables and their spatial and temporal derivatives. The approximation can be carried out successively to obtain the Euler, Navier–Stokes, Burnett equations, and so on. A vast majority of practical applications can be satisfactorily described by the Navier–Stokes equation, especially for single-phase large-scale Newtonian flows. However, deficiencies appear in more complex and general flow regimes involving multiple phases, high Mach numbers, or high Knudsen numbers. In those situations, higher-order hydrodynamic descriptions become necessary. Unfortunately, the complexity of the Chapman-Enskog calculation increases tremendously as the order of approximation increases, yielding highly nonlinear high-order partial differential equations. Worse still, it is well-known that the higher-order corrections in the gradient expansion to the Navier–Stokes equations are ill-posed and many questions about the meaningfulness of the Chapman-Enskog solutions to the Boltzmann equations have been raised (Cercignani 1975; Ernst *et al.* 1978). Mode-coupling theories (Ernst & Dorfman 1975; Ernst *et al.* 1978) and computer simulations (Standish 1999) have revealed that the transport coefficients corresponding to the Burnett and super-Burnett terms actually diverge in the thermodynamic limit, indicating non-analytic (in the gradients) corrections.

In an alternative approach, Grad (1949*b*, 1952) proposed to approximate the Boltzmann equation by expanding the single-particle distribution function on the basis of the Hermite orthogonal polynomials in velocity space. The Hermite polynomials are chosen because the expansion coefficients are exactly the velocity moments of the distribution function. The truncation of higher-order terms in a Hermite expansion do not directly alter the velocity moments of the distribution function. The resulting equations for the Hermite coefficients are directly constructed out of projecting Boltzmann equation onto a truncated Hermite polynomial basis using the standard Galerkin procedure. Grad kept thirteen of the leading Hermite coefficients, essentially the five fundamental thermohydrodynamic variables (mass density, fluid velocity and internal energy) and their fluxes, as the state variables and obtained a closed system of partial differential equations known as the Grad 13-moment system. It has been shown that this description contains far more physics than that in the Navier–Stokes (see Gad-el-Hak 1999; Agarwal, Yun & Balakrishnan 2001). Unfortunately, the Grad 13-moment equations are just as complicated and difficult to solve as those obtained by higher-order Chapman-Enskog expansions.

Quite independent of the continuum kinetic theory, the lattice Boltzmann methods (LBM) (McNamara & Zanetti 1988; Benzi, Succi & Vergassola 1992; Qian, d'Humieres & Lallemand 1992; Chen, Chen & Matthaeus 1992*a*; Chen & Doolen 1998) originated from lattice gas cellular automaton models (Frisch, Hasslacher &

Pomeau 1986; Wolfram 1986; Doolen 1989). Over the decade since its conception, LBM has quickly been shown to be an accurate and efficient method for computational fluid dynamics (CFD) simulations (Chen *et al.* 1992*b*; Martínez *et al.* 1994; Hou *et al.* 1995; Shan 1997; Chen *et al.* 1998). Comparing with traditional CFD methods, the LBM method is easy to implement, intrinsically parallelizable, and handles complex boundary conditions well. More importantly, owing to its kinetic nature, the LBM method allows the microscopic physics responsible for many complex fluid phenomena to be modelled more directly (Shan & Chen 1993, 1994; Shan & Doolen 1995; Nekovee *et al.* 2000; Chin, Boek & Coveney 2002; Sankaranarayanan *et al.* 2002). However, the original LBM formulations of Qian *et al.* (1992) and Chen *et al.* (1992*a*) do not provide a systematic way of deriving lattice Boltzmann models, particularly when thermohydrodynamics involving a conserved energy degree of freedom is considered (Alexander, Chen & Sterling 1993; McNamara & Alder 1993; Chen, Ohashi & Akiyama 1994; Chen, Teixeira & Molvig 1997). Instead, the equilibrium distribution function is chosen as a polynomial form in power of fluid velocity with the coefficients determined *a posteriori* by requiring that the resulting first-order Chapman-Enskog expansion must recover the Navier–Stokes equation. Although it was later pointed out by Abe (1997) and He & Luo (1997) that the equilibrium distribution function is, in fact, small velocity expansions of the Maxwell–Boltzmann distribution, and the discrete velocities are, in fact, the abscissae of Gaussian–Hermite quadratures to ensure accurate evaluation of leading moments of the distribution, there is no rigorous and systematic way of formulating models that accomplish higher-order hydrodynamic physics. In fact, the present LBM approach has not been extended beyond the level of the Navier–Stokes. This has generated some confusion and misstatements in the community, such as that LBM is only valid for Navier–Stokes hydrodynamics.

Inspired by Grad's original work, Shan & He (1998) proposed a new theoretical approach for discretizing the Boltzmann-BGK equation in velocity space which relates the lattice Boltzmann method to the Grad 13-moment system. Truncation of the Hermite expansion of the Boltzmann distribution function is seen as equivalent to solving the Boltzmann-BGK equation for selected discrete microscopic velocity values. Thus, a purely kinetic description of fluid systems equivalent to that obtained through Grad's expansion procedure is obtained. Contrary to Grad's approach, the discrete values of the distribution function instead of the moment integrals are used as the state variables, resulting in a much simpler set of governing equations that is kinetic in nature and uniform in form. As a result, higher approximations to the Boltzmann equation beyond the Navier–Stokes level can be constructed easily in this representation by merely expanding the equilibrium distribution to higher orders and adopting quadratures of a sufficiently high degree of precision.

In this paper, we discuss the kinetic representation in detail. In § 2, we first provide the necessary basic background in kinetic theory for the continuum Boltzmann equation. We show how the conventional fluid quantities are related to the moment integrals of the Boltzmann distributions. In § 3, we give a detailed description of the new theoretical formulation in terms of expanding the Boltzmann equation onto the Hermite basis. We demonstrate how the truncated Hermite basis is related to the sufficient conditions for the requirements of the thermal and isothermal Navier–Stokes fluids as well as higher-orders extensions. We show how the discretization of the velocity space is directly related to the hydrodynamic moment integrations via the Gauss–Hermite quadrature. In § 4, we show how various levels of truncations in the Hermite basis correspond to the accuracy requirements in describing fluid dynamic properties that are associated with the degrees in non-equilibrium Boltzmann distribution functions. This establishes a general rule for systematically formulating models that are sufficient for the Navier–Stokes, Burnett fluids and beyond. In § 5, we demonstrate that the popular lattice Boltzmann models can be derived as special examples. Moreover, we describe how to go beyond the Navier–Stokes equation and present some relevant high-order lattice Boltzmann models. Concluding remarks and discussions are given in § 6. An Appendix on the mathematical details is also provided for the sake of completeness.

2. Basic background–continuum Boltzmann-BGK equation

Without loss of generality, we consider a fluid system in D-dimensional space. Let $\boldsymbol{x}$ be the Cartesian coordinates of the configuration space and $\boldsymbol{\xi}$ that of the velocity space. The single particle distribution function, $f(\boldsymbol{\xi}, \boldsymbol{x}, t)$, is defined such that $f(\boldsymbol{\xi}, \boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{\xi}\,\mathrm{d}\boldsymbol{x}$ represents the number of particles in the phase space element $\mathrm{d}\boldsymbol{\xi}\,\mathrm{d}\boldsymbol{x}$ at time t.

The distribution function contains more detailed information about the fluid system than the macroscopic thermodynamic variables do, as by definition, the latter are the low-order moment integrals of f in velocity space. Specifically, the number density, $n(\boldsymbol{x}, t)$, the mass density, $\rho(\boldsymbol{x}, t) \equiv mn(\boldsymbol{x}, t)$, where m is the molecular mass of gas particles, the fluid velocity, $\boldsymbol{u}(\boldsymbol{x}, t)$ and the kinetic energy density per unit mass, $\epsilon(\boldsymbol{x}, t)$, are defined, respectively, as:

$$\rho(\boldsymbol{x}, t) \equiv mn(\boldsymbol{x}, t) = m \int f\,\mathrm{d}\boldsymbol{\xi}, \tag{2.1a}$$

$$\rho\boldsymbol{u}(\boldsymbol{x}, t) = m \int f\boldsymbol{\xi}\,\mathrm{d}\boldsymbol{\xi}, \tag{2.1b}$$

$$\rho\epsilon(\boldsymbol{x}, t) = \tfrac{1}{2}m \int f|\boldsymbol{\xi} - \boldsymbol{u}|^2\,\mathrm{d}\boldsymbol{\xi}. \tag{2.1c}$$

These are the conventional hydrodynamic variables corresponding to the basic conservation laws of mass, momentum and energy. Also of great physical significance are the second and third moments which are more conveniently considered in the reference frame moving with the bulk of the fluid flow. Introducing the *intrinsic velocity*, $\boldsymbol{c} = \boldsymbol{\xi} - \boldsymbol{u}(\boldsymbol{x}, t)$, the full second and third moments are defined, respectively, by:

$$P_{ij} = m \int f c_i c_j\,\mathrm{d}\boldsymbol{c}, \qquad Q_{ijk} = m \int f c_i c_j c_k\,\mathrm{d}\boldsymbol{c}, \tag{2.2}$$

where the subscripts i, j, k denote Cartesian components. Here and throughout this manuscript, we shall use vector and component notations for tensors interchangeably. Einstein summation convention is implied for any repeated indices in the component notation.

In the reference frame moving with the fluid, the component of the momentum flux tensor, P_{ij}, represents the rate of momentum transfer of the i-component in the j-direction. Ignoring long-range intermolecular interactions, the hydrodynamic pressure, p, can be found as the average of the diagonal components of P_{ij}: $p = P_{ii}/D = 2\rho\epsilon/D$. The traceless stress tensor $\boldsymbol{\sigma}$ is defined as:

$$\sigma_{ij} = P_{ij} - p\delta_{ij}, \tag{2.3}$$

where δ_{ij} is the Kronecker delta function. For a monatomic ideal gas in D-dimensions, the temperature, θ, is related to the internal energy density $\rho\epsilon$ by:

$$\rho\epsilon = \frac{D}{2} n k_B \theta \quad \text{or} \quad \epsilon = \frac{D k_B \theta}{2m}, \tag{2.4}$$

where k_B is the Boltzmann constant. Thus, we have the ideal-gas equation of state:

$$p = n k_B \theta. \tag{2.5}$$

The contracted third moment component,

$$\tfrac{1}{2} q_i \equiv \tfrac{1}{2} Q_{ijj} = \frac{m}{2} \int f c^2 c_i \,\mathrm{d}\boldsymbol{c}, \tag{2.6}$$

is by definition the rate of heat transfer due to the molecular motion.

The evolution of the single-particle distribution function obeys the Boltzmann equation. For simplicity, we describe the analytical formulation based on the BGK collision model. As our starting point, f satisfies the following equation (often known as the Krook equation):

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla f + \boldsymbol{g} \cdot \nabla_{\xi} f = -\frac{1}{\tau} \left[f - f^{(0)} \right]. \tag{2.7}$$

Here, τ is the characteristic relaxation time of collisions to equilibrium, ∇_ξ the gradient operator in velocity space, and $\boldsymbol{g}$ the acceleration from the external or self-generated body-force field. $f^{(0)}$ represents a local equilibrium distribution (i.e. Maxwell–Boltzmann) in the reference frame moving with the bulk of the flow:

$$f^{(0)} = \rho \left(\frac{m}{2\pi k_B \theta} \right)^{D/2} \exp\left[-\frac{m c^2}{2 k_B \theta} \right]. \tag{2.8}$$

For convenience, we choose the characteristic velocity to be $c_0 \equiv \sqrt{k_B \theta_0 / m_0}$, where θ_0 and m_0 are, respectively, the characteristic temperature and the unit of mass of the gas molecules, which in a single-component gas can be chosen simply as the molecular mass of the gas particles. c_0 is easily recognized as the *sound speed* at temperature θ_0. On scaling all velocities with respect to c_0 and choosing the characteristic length and time scales, l_0 and t_0 respectively, such that $l_0 = c_0 t_0$, all equations above remain unchanged except that (2.5) becomes $p = \rho\theta$ and (2.8) takes the following simpler dimensionless form:

$$f^{(0)} = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left[-\frac{c^2}{2\theta} \right]. \tag{2.9}$$

Hereinafter (2.1) and (2.7) are to be understood as dimensionless with all velocities, $\boldsymbol{\xi}$, $\boldsymbol{u}$ and $\boldsymbol{c}$, measured in the units of c_0. Of course, at constant temperature $\theta = 1$, the sound speed in the gas system is unity. We shall return to the topic of scaling when devising a computation scheme by discretizing space and time.

Equations (2.1), (2.7) and (2.9) are a closed set of integro-differential equations. Their solution gives the full time history of the $(2D)$-dimensional single particle distribution function. For most practical purposes this is not only computationally too expensive, but is also unnecessary. The fundamental hydrodynamic variables corresponding to the first few moments of the distribution function (equations (2.1)) are sufficient to describe macroscopic flow properties. Their governing equations can be constructed by taking the moments of (2.7). Using the fact that the moment integrals of (2.1) lead to the vanishing right-hand side of (2.7) and after some straightforward algebraic manipulations, we arrive at the following familiar conservation equations for mass, momentum and total energy:

$$\frac{\partial\rho}{\partial t}+\frac{\partial\rho u_i}{\partial x_i}=0, \tag{2.10a}$$

$$\rho\frac{\mathrm{d}u_i}{\mathrm{d}t}+\frac{\partial P_{ij}}{\partial x_j}=\rho g_i, \tag{2.10b}$$

$$\rho\frac{\mathrm{d}\epsilon}{\mathrm{d}t}+P_{ij}\frac{\partial u_i}{\partial x_j}+\frac{1}{2}\frac{\partial q_i}{\partial x_i}=0, \tag{2.10c}$$

where,

$$\frac{\mathrm{d}}{\mathrm{d}t}=\frac{\partial}{\partial t}+u_i\frac{\partial}{\partial x_i} \tag{2.11}$$

is the Lagrangian derivative. Though exact, the above equations are not closed because of the appearance of high-order moments, P_{ij} and q_i, in the equations for lower-order moments.

In the Chapman–Enskog approximation (Chapman & Cowling 1970), approximations to the distribution function f in terms of hydrodynamic variables and their derivatives are obtained successively. With the BGK collision model, the Chapman-Enskog procedure of obtaining hydrodynamic equations is greatly simplified (see Huang 1987). It is critical to notice that the forms of the macroscopic equations obtained through such a procedure only depend on the leading moments of the distribution function instead of the full form of the distribution function. Consequently, truncation of the higher-order terms in the Hermite expansion of the distribution function has no explicit effect on the macroscopic equations. We shall return to this point later.

Alternative to the Chapman–Enskog procedure, in a series of papers published more than half a century ago, Grad (1949*b*, 1952) argued that the fluid equations obtained above cannot be sufficient for all purposes and suggested that the stress tensor and the heat flux be treated on an equal footing with the conventional thermohydrodynamic variables. He obtained a set of partial differential equations for the thirteen most significant moments, namely ρ, $\boldsymbol{u}$, θ, σ_{ij} and q_i, by expanding the Boltzmann distribution function in terms of Hermite polynomials. In the next section, by applying the same Hermite expansion technique and noticing the correspondence between the Hermite expansion coefficients of a Hermite-truncated function and the function values at a special set of discrete velocities, we can approximate the Boltzmann-BGK equation by a small set of discrete kinetic equations. The approximation is essentially equivalent to that employed in the Grad 13-moment system. Better still, it produces a set of uniform kinetic equations that permit easy extension to higher-degree approximations.

3. Projecting Boltzmann-BGK onto Hermite basis

3.1. *Moments and truncated Hermite series*

We seek solutions to (2.1), (2.7) and (2.9) by expanding $f(\boldsymbol{x},\boldsymbol{\xi},t)$ in Hermite (Gram–Charlier) polynomials. The mathematical property of the Hermite polynomials, especially that in higher dimensions, has been extensively treated by Grad (1949*a*). As demonstrated below, a unique feature in using the Hermite polynomials as the expansion basis rather than any other functions is that the expansion coefficients correspond precisely to the velocity moments up to the given degrees. Some necessary mathematical knowledge is summarized in the Appendix.

Following the standard procedure, we expand the distribution function f in terms of the dimensionless Hermite ortho-normal polynomials in velocity space $\boldsymbol{\xi}$:

$$f(\boldsymbol{x}, \boldsymbol{\xi}, t) = \omega(\boldsymbol{\xi}) \sum_{n=0}^{\infty} \frac{1}{n!} \boldsymbol{a}^{(n)}(\boldsymbol{x}, t) \mathscr{H}^{(n)}(\boldsymbol{\xi}). \tag{3.1}$$

Note that both $\boldsymbol{a}^{(n)}$ and $\mathscr{H}^{(n)}$ are rank-n tensors and the product on the right-hand side denotes full contraction. The dimensionless expansion coefficients, $\boldsymbol{a}^{(n)}(\boldsymbol{x}, t)$, are given by

$$\boldsymbol{a}^{(n)}(\boldsymbol{x}, t) = \int f(\boldsymbol{x}, \boldsymbol{\xi}, t) \mathscr{H}^{(n)}(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi}, \tag{3.2}$$

where the integration is carried over the entire dimensionless velocity space of $\boldsymbol{\xi}$.

Evidently from (3.2), all the expansion coefficients are linear combinations of the velocity moments of f. Specifically, on substituting the explicit expressions of the Hermite polynomials (equations (A 3)) into (3.2), the first few expansion coefficients are directly identified with the familiar hydrodynamic variables:

$$\boldsymbol{a}^{(0)} = \int f \, \mathrm{d}\boldsymbol{\xi} = \rho, \tag{3.3a}$$

$$\boldsymbol{a}^{(1)} = \int f \boldsymbol{\xi} \, \mathrm{d}\boldsymbol{\xi} = \rho \boldsymbol{u}, \tag{3.3b}$$

$$\boldsymbol{a}^{(2)} = \int f(\boldsymbol{\xi}^2 - \boldsymbol{\delta}) \, \mathrm{d}\boldsymbol{\xi} = \boldsymbol{P} + \rho(\boldsymbol{u}^2 - \boldsymbol{\delta}), \tag{3.3c}$$

$$\boldsymbol{a}^{(3)} = \int f(\boldsymbol{\xi}^3 - \boldsymbol{\xi}\boldsymbol{\delta}) \, \mathrm{d}\boldsymbol{\xi}, = \boldsymbol{Q} + \boldsymbol{u}\boldsymbol{a}^{(2)} - (D-1)\rho \boldsymbol{u}^3. \tag{3.3d}$$

Here and throughout the manuscript, we have adopted the shorthand notations of Grad (1949*a*) for fully symmetric tensors. The product of two tensors always means the sum of all possible permutations of tensor product. For instance, $\boldsymbol{u}\boldsymbol{a}^{(2)}$ stands for $u_i a_{jk}^{(2)} + u_j a_{ik}^{(2)} + u_k a_{ij}^{(2)}$. In addition, the power of a vector such as $\boldsymbol{u}^3$ denotes the direct vector products $\boldsymbol{uuu}$ which is not to be confused with the power of the norm of the vector, u^3.

Evidently, the thermohydrodynamic variables can be expressed in terms of the low-order Hermite expansion coefficients:

$$\rho = \boldsymbol{a}^{(0)}, \tag{3.4a}$$

$$\rho \boldsymbol{u} = \boldsymbol{a}^{(1)}, \tag{3.4b}$$

$$\boldsymbol{P} = \boldsymbol{a}^{(2)} - \rho(\boldsymbol{u}^2 - \boldsymbol{\delta}), \tag{3.4c}$$

$$\boldsymbol{Q} = \boldsymbol{a}^{(3)} - \boldsymbol{u}\boldsymbol{a}^{(2)} + (D-1)\rho \boldsymbol{u}^3, \tag{3.4d}$$

while the internal energy is:

$$\rho \epsilon = \tfrac{1}{2}\left[a_{ii}^{(2)} - \rho(u^2 - D)\right]. \tag{3.5}$$

Therefore, the five fundamental thermohydrodynamic variables, ρ, $\boldsymbol{u}$ and θ $(= 2\epsilon/D)$, and the momentum flux tensor $\boldsymbol{P}$ (or its traceless part, the stress tensor $\boldsymbol{\sigma}$) are completely determined by the first three Hermite expansion coefficients alone, whereas the third moment, i.e. the heat flux $\boldsymbol{q}$, is completely determined by the fourth coefficient.

Owing to the mutual orthogonality of Hermite polynomials, the leading moments of a distribution function up to Nth order are preserved by truncations of the higher-order terms in its Hermite expansion. Consequently, a distribution function can be approximated by its projection onto a Hilbert subspace spanned by the first N Hermite polynomials without changing the first N moments, i.e.

$$f(\boldsymbol{x}, \boldsymbol{\xi}, t) \approx f^N(\boldsymbol{x}, \boldsymbol{\xi}, t) = \omega(\boldsymbol{\xi}) \sum_{n=0}^{N} \frac{1}{n!} \boldsymbol{a}^{(n)}(\boldsymbol{x}, t) \mathscr{H}^{(n)}(\boldsymbol{\xi}). \tag{3.6}$$

Here, up to Nth order, $f^N(\boldsymbol{x}, \boldsymbol{\xi}, t)$ has exactly the same velocity moments as the original $f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ does. This guaranties that a fluid dynamic system can be constructed by a finite set of macroscopic variables (thermohydrodynamic moments). Indeed, in Grad's 13-moment system, the governing differential equations for the basic thermohydrodynamic variables $(\rho, \boldsymbol{u}, \theta)$ and their fluxes are derived from a properly truncated Hermite expansion.

3.2. *Discretization of velocity space*

Instead of formulating a macroscopic descriptions in terms of thermohydrodynamic variables, we seek approximations to the Boltzmann-BGK equation, i.e. (2.7), by remaining in the kinetic level of representation via suitable truncated Hermite expansions. It is crucial to realize that as a partial sum of Hermite series with finite terms, the truncated distribution function of (3.6) can be completely and uniquely determined by its values at a set of discrete abscissae. This is true because with f truncated to order N, the integrand on the right-hand side of (3.2) can be written as:

$$f^N(\boldsymbol{x}, \boldsymbol{\xi}, t) \mathscr{H}^{(n)}(\boldsymbol{\xi}) = \omega(\boldsymbol{\xi}) p(\boldsymbol{x}, \boldsymbol{\xi}, t), \tag{3.7}$$

where $p(\boldsymbol{x}, \boldsymbol{\xi}, t)$ is a polynomial in $\boldsymbol{\xi}$ of a degree not greater than $2N$. Using the Gauss–Hermite quadrature (c.f. the Appendix), $\boldsymbol{a}^{(n)}$ in (3.2) can be precisely expressed as a weighted sum of the functional values of $p(\boldsymbol{x}, \boldsymbol{\xi}, t)$:

$$\boldsymbol{a}^{(n)} = \int \omega(\boldsymbol{\xi}) p(\boldsymbol{x}, \boldsymbol{\xi}, t) \, \mathrm{d}\boldsymbol{\xi} = \sum_{a=1}^{d} w_a p(\boldsymbol{x}, \boldsymbol{\xi}_a, t) = \sum_{a=1}^{d} \frac{w_a}{\omega(\boldsymbol{\xi}_a)} f^N(\boldsymbol{x}, \boldsymbol{\xi}_a, t) \mathscr{H}^{(n)}(\boldsymbol{\xi}_a), \tag{3.8}$$

where w_a and $\boldsymbol{\xi}_a$, $a = 1, \ldots, d$, are, respectively, the weights and abscissae of a Gauss–Hermite quadrature of a degree $\geqslant 2N$. Hence, the set of discrete function values, $\{f^N(\boldsymbol{x}, \boldsymbol{\xi}_a, t) \, : \, a = 1, \ldots, d\}$, completely determines f^N and therefore its first N velocity moments, and vice versa. The discrete distribution function values $f^N(\boldsymbol{\xi}_a)$ can serve as a new set of fundamental variables for defining the fluid system in place of the conventional thermohydrodynamic variables. That is, as long as $f^N(\boldsymbol{\xi}_a)$ are known, the system is known to the same level of detail as defined by the first N fundamental thermohydrodynamic moments.

The governing equations for $f^N(\boldsymbol{\xi}_a)$ can be obtained by projecting (2.7) on a Hermite-truncated basis and evaluating at $\boldsymbol{\xi}_a$. This can be accomplished term by term in (2.7). First, the Maxwell–Boltzmann distribution $f^{(0)}$ on the right-hand side of (2.7) must be truncated according to (3.6). Let $\boldsymbol{a}_0^{(n)}$ be the nth Hermite coefficient of $f^{(0)}$. Using (3.2), we have

$$\boldsymbol{a}_0^{(n)} = \int f^{(0)} \mathscr{H}^{(n)}(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi}. \tag{3.9}$$

Notice from (2.9) and (A 1) that

$$f^{(0)} = \frac{\rho}{(\sqrt{\theta})^D}\omega\left(\frac{\boldsymbol{\xi}-\boldsymbol{u}}{\sqrt{\theta}}\right), \tag{3.10}$$

after a change of the dummy variable $(\boldsymbol{\xi}-\boldsymbol{u})/\sqrt{\theta} \to \boldsymbol{\eta}$, we have

$$\boldsymbol{a}_0^{(n)} = \rho \int \omega(\boldsymbol{\eta})\mathscr{H}^{(n)}(\sqrt{\theta}\boldsymbol{\eta}+\boldsymbol{u})\,\mathrm{d}\boldsymbol{\eta}. \tag{3.11}$$

Using (A 3), the leading Hermite coefficients of the Maxwellian are obtained as:

$$\boldsymbol{a}_0^{(0)} = \rho, \tag{3.12a}$$

$$\boldsymbol{a}_0^{(1)} = \rho\boldsymbol{u}, \tag{3.12b}$$

$$\boldsymbol{a}_0^{(2)} = \rho[\boldsymbol{u}^2 + (\theta-1)\boldsymbol{\delta}], \tag{3.12c}$$

$$\boldsymbol{a}_0^{(3)} = \rho[\boldsymbol{u}^3 + (\theta-1)\boldsymbol{\delta}\boldsymbol{u}], \tag{3.12d}$$

$$\boldsymbol{a}_0^{(4)} = \rho[\boldsymbol{u}^4 + (\theta-1)\boldsymbol{\delta}\boldsymbol{u}^2 + (\theta-1)^2\boldsymbol{\delta}^2]. \tag{3.12e}$$

The explicit Hermite expansion of the Maxwellian $f^{(0)}$ is therefore:

$$f^{(0)}(\boldsymbol{\xi}) = \omega(\boldsymbol{\xi})\rho\left\{1 + \boldsymbol{\xi}\cdot\boldsymbol{u} + \underbrace{\tfrac{1}{2}[(\boldsymbol{\xi}\cdot\boldsymbol{u})^2 - u^2 + (\theta-1)(\xi^2-D)]}_{\text{2nd order}}\right.$$
$$\left. + \underbrace{\frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{6}[(\boldsymbol{\xi}\cdot\boldsymbol{u})^2 - 3u^2 + 3(\theta-1)(\xi^2-D-2)]}_{\text{3rd order}}\right\}. \tag{3.13}$$

Notice, all the terms proportional to $\theta-1$ vanish for an ‘isothermal’ system in which $\theta=1$.

3.3. *Formulation of the body-force term*

The third term on the left-hand side of (2.7) represents the effect of body forces and should also be projected onto the truncated Hermite basis. However, this term involves derivatives in $\boldsymbol{\xi}$ and cannot be expressed directly using the values of the distribution function alone. Fortunately, its Hermite expansion can be obtained from the expansion of f by taking the derivative of (3.1) and using (A 2) repeatedly (Martys, Shan & Chen 1998):

$$\begin{aligned}\nabla_\xi f &= \sum_{n=0}^{\infty}\frac{1}{n!}\boldsymbol{a}^{(n)}\nabla_\xi\left(\omega\mathscr{H}^{(n)}\right) = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\boldsymbol{a}^{(n)}\nabla_\xi^{n+1}\omega \\ &= -\omega\sum_{n=0}^{\infty}\frac{1}{n!}\boldsymbol{a}^{(n)}\mathscr{H}^{(n+1)} = -\omega\sum_{n=1}^{\infty}\frac{1}{n!}n\boldsymbol{a}^{(n-1)}\mathscr{H}^{(n)}.\end{aligned} \tag{3.14}$$

Defining $F(\boldsymbol{\xi}) \equiv -\boldsymbol{g}\cdot\nabla_\xi f$, we have the following Hermite expansion of the body force term:

$$F(\boldsymbol{\xi}) = \omega\sum_{n=1}^{\infty}\frac{1}{n!}\boldsymbol{g}\boldsymbol{a}^{(n-1)}\mathscr{H}^{(n)}, \tag{3.15}$$

where, $\boldsymbol{g}\boldsymbol{a}^{(n-1)}$ denotes the symmetric tensor product of $\boldsymbol{g}$ and $\boldsymbol{a}^{(n-1)}$. Once again, Grad's short-hand notation is used here to designate the sum of all n permutations of tensor product between $\boldsymbol{g}$ and $\boldsymbol{a}^{(n-1)}$ by $\boldsymbol{g}\boldsymbol{a}^{(n-1)}$.

Since the leading Hermite coefficients of f are given by (3.3), we have

$$\boldsymbol{a}^{(0)} = \boldsymbol{a}_0^{(0)}, \quad \boldsymbol{a}^{(1)} = \boldsymbol{a}_0^{(1)}, \quad \boldsymbol{a}^{(2)} = \boldsymbol{a}_0^{(2)} + \boldsymbol{\sigma}, \tag{3.16}$$

where $\boldsymbol{\sigma}$ is the stress tensor defined in (2.3). Thus, the expression for $F(\boldsymbol{\xi})$ can be determined order by order. For terms up to the third order, it explicitly gives:

$$F(\boldsymbol{\xi}) = \omega(\boldsymbol{\xi})\rho \left\{ \underbrace{\boldsymbol{g}\cdot\boldsymbol{\xi}}_{\text{1st}} + \underbrace{(\boldsymbol{g}\cdot\boldsymbol{\xi})(\boldsymbol{u}\cdot\boldsymbol{\xi}) - \boldsymbol{g}\cdot\boldsymbol{u}}_{\text{2nd order}} + \underbrace{\frac{1}{2\rho}a^{(2)}\left[(\boldsymbol{g}\cdot\boldsymbol{\xi})\mathscr{H}^{(2)}(\boldsymbol{\xi}) - 2\boldsymbol{g}\boldsymbol{\xi}\right]}_{\text{3rd order}} \right\}. \tag{3.17}$$

3.4. *Boltzmann-BGK with discrete velocities*

We are now ready to obtain the governing equations for $f^N(\boldsymbol{\xi}_a)$. Hereinafter, we shall omit the superscript N, and the distribution function is understood to be restricted in the truncated subspace. Applying Gauss–Hermite quadrature to (2.1) gives:

$$\rho = \sum_{a=1}^{d} \frac{w_a f(\boldsymbol{\xi}_a)}{\omega(\boldsymbol{\xi}_a)}, \tag{3.18a}$$

$$\rho\boldsymbol{u} = \sum_{a=1}^{d} \frac{w_a f(\boldsymbol{\xi}_a)\boldsymbol{\xi}_a}{\omega(\boldsymbol{\xi}_a)}, \tag{3.18b}$$

$$\boldsymbol{P} + \rho\boldsymbol{u}^2 = \sum_{a=1}^{d} \frac{w_a f(\boldsymbol{\xi}_a)\boldsymbol{\xi}_a\boldsymbol{\xi}_a}{\omega(\boldsymbol{\xi}_a)}. \tag{3.18c}$$

The trace of the last equation yields:

$$\rho(D\theta + u^2) = \sum_{a=1}^{d} \frac{w_a f(\boldsymbol{\xi}_a)\xi_i^2}{\omega(\boldsymbol{\xi}_a)}. \tag{3.19}$$

Defining $f_a(\boldsymbol{x}, t) = w_a f(\boldsymbol{x}, \boldsymbol{\xi}_a, t)/\omega(\boldsymbol{\xi}_a)$, for $a = 1, \ldots, d$, the above equations become:

$$\rho = \sum_{a=1}^{d} f_a, \tag{3.20a}$$

$$\rho\boldsymbol{u} = \sum_{a=1}^{d} f_a\boldsymbol{\xi}_a, \tag{3.20b}$$

$$\boldsymbol{P} + \rho\boldsymbol{u}\boldsymbol{u} = \sum_{a=1}^{d} f_a\boldsymbol{\xi}_a\boldsymbol{\xi}_a, \tag{3.20c}$$

$$\rho(D\theta + u^2) = \sum_{a=1}^{d} f_a\xi_a^2. \tag{3.20d}$$

Next, after moving the body force term to the right-hand side, (2.7) becomes:

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi}\cdot\nabla f = -\frac{1}{\tau}\left[f - f^{(0)}\right] + F(\boldsymbol{\xi}). \tag{3.21}$$

By directly evaluating at $\boldsymbol{\xi}_a$ and multiplying by the constants $w_a/\omega(\boldsymbol{\xi}_a)$, we obtain the following equations for f_a:

$$\frac{\partial f_a}{\partial t} + \boldsymbol{\xi}_a \cdot \nabla f_a = -\frac{1}{\tau}\left[f_a - f_a^{(0)}\right] + F_a \quad (a = 1, \dots, d), \tag{3.22}$$

where on the right-hand side,

$$f_a^{(0)} \equiv \frac{w_a}{\omega(\boldsymbol{\xi}_a)} f^{(0)}(\boldsymbol{\xi}_a) = w_a \rho \left\{ 1 + \underbrace{\boldsymbol{\xi}_a \cdot \boldsymbol{u}}_{\text{1st order}} + \underbrace{\tfrac{1}{2}\left[(\boldsymbol{\xi}_a \cdot \boldsymbol{u})^2 - u^2 + (\theta - 1)\left(\xi_a^2 - D\right)\right]}_{\text{2nd order}} \right.$$
$$\left. + \underbrace{\frac{\boldsymbol{\xi}_a \cdot \boldsymbol{u}}{6}\left[(\boldsymbol{\xi}_a \cdot \boldsymbol{u})^2 - 3u^2 + 3(\theta - 1)\left(\xi_a^2 - D - 2\right)\right]}_{\text{3rd order}} + \cdots \right\}, \tag{3.23}$$

and

$$F_a \equiv \frac{w_a}{\omega(\boldsymbol{\xi}_a)} F(\boldsymbol{\xi}_a) = w_a \rho \left\{ \underbrace{\boldsymbol{\xi}_a \cdot \boldsymbol{g}}_{\text{1st order}} + \underbrace{(\boldsymbol{\xi}_a \cdot \boldsymbol{g})(\boldsymbol{\xi}_a \cdot \boldsymbol{u}) - \boldsymbol{g} \cdot \boldsymbol{u}}_{\text{2nd order}} \right.$$
$$\left. + \underbrace{\frac{1}{2\rho} a^{(2)}\left[(\boldsymbol{\xi}_a \cdot \boldsymbol{g})\mathscr{H}^{(2)}(\boldsymbol{\xi}_a) - 2\boldsymbol{g}\boldsymbol{\xi}_a\right]}_{\text{3rd order}} + \cdots \right\}. \tag{3.24}$$

Note that in (3.24), the first- and second-order terms do not depend on the non-equilibrium properties in f_a. However, the third-order terms and those beyond do involve the information of the full f_a.

It is convenient to absorb the body force term of (3.24) into $f_a^{(0)}$ in (3.22) to form an effective equilibrium distribution $f_a^{(eq)} \equiv f_a^{(0)} + \tau F_a$, so that we can write

$$\frac{\partial f_a}{\partial t} + \boldsymbol{\xi}_a \cdot \nabla f_a = -\frac{1}{\tau}\left[f_a - f_a^{(eq)}\right]. \tag{3.25}$$

Combining (3.1) and (3.15), $f^{(eq)}$ has the following Hermite expansion:

$$f^{(eq)} = \omega \sum_{n=1}^{\infty} \frac{1}{n!}\left[\boldsymbol{a}_0^{(n)} + \tau \boldsymbol{g}\boldsymbol{a}^{(n-1)}\right]\mathscr{H}^{(n)}. \tag{3.26}$$

Using (3.12) and (3.16), the leading expansion coefficients of $f^{(eq)}$, noted by $\boldsymbol{a}_{eq}^{(n)}$, are:

$$\boldsymbol{a}_{eq}^{(0)} = \rho, \tag{3.27a}$$
$$\boldsymbol{a}_{eq}^{(1)} = \rho[\boldsymbol{u} + \tau \boldsymbol{g}], \tag{3.27b}$$
$$\boldsymbol{a}_{eq}^{(2)} = \rho[\boldsymbol{u}^2 + \tau \boldsymbol{g}\boldsymbol{u} + (\theta - 1)\boldsymbol{\delta}], \tag{3.27c}$$
$$\boldsymbol{a}_{eq}^{(3)} = \rho[\boldsymbol{u}^3 + \tau \boldsymbol{g}\boldsymbol{u}^2 + (\theta - 1)\boldsymbol{\delta}(\boldsymbol{u} + \tau \boldsymbol{g})] + \tau \boldsymbol{g}\boldsymbol{\sigma}. \tag{3.27d}$$

If we define a 'post-collide' velocity $\boldsymbol{u}' = \boldsymbol{u} + \tau \boldsymbol{g}$, it is straightforward to rewrite the above as:

$$\boldsymbol{a}_{eq}^{(0)} = \boldsymbol{a}_0^{(0)}(\rho, \boldsymbol{u}', \theta), \tag{3.28a}$$
$$\boldsymbol{a}_{eq}^{(1)} = \boldsymbol{a}_0^{(1)}(\rho, \boldsymbol{u}', \theta), \tag{3.28b}$$

$$\boldsymbol{a}_{eq}^{(2)} = \boldsymbol{a}_0^{(2)}(\rho, \boldsymbol{u}', \theta) - \rho\tau^2\boldsymbol{g}^2, \tag{3.28c}$$

$$\boldsymbol{a}_{eq}^{(3)} = \boldsymbol{a}_0^{(3)}(\rho, \boldsymbol{u}', \theta) - \rho\tau^2\boldsymbol{g}^2\boldsymbol{u} - \rho\tau^3\boldsymbol{g}^3 + \tau\boldsymbol{g}\boldsymbol{\sigma}. \tag{3.28d}$$

Therefore, the 'effective' equilibrium distribution is the Maxwellian distribution with a local velocity of $\boldsymbol{u}'$, plus a high-order correction f':

$$f_a^{(eq)} = f_a^{(0)}(\rho, \boldsymbol{u}', \theta) + f_a'. \tag{3.29}$$

Using (3.28), f_a' can be written explicitly as:

$$f_a' = \rho\tau^2[g^2 - (\boldsymbol{g}\cdot\boldsymbol{\xi}_i)^2] + \rho\tau^2\left\{\frac{(\boldsymbol{u}\cdot\boldsymbol{\xi}_i)}{2}[g^2 - (\boldsymbol{g}\cdot\boldsymbol{\xi}_i)^2] + (\boldsymbol{g}\cdot\boldsymbol{\xi}_i)(\boldsymbol{g}\cdot\boldsymbol{u})\right\}$$
$$+ \tfrac{1}{6}\rho\tau^3(\boldsymbol{g}\cdot\boldsymbol{\xi}_i)[3g^2 - (\boldsymbol{g}\cdot\boldsymbol{\xi}_i)^2] + \tau\left[\frac{(\boldsymbol{g}\cdot\boldsymbol{\xi}_i)}{2}\boldsymbol{\sigma}:\boldsymbol{\xi}_a\boldsymbol{\xi}_a - \boldsymbol{g}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{\xi}_a\right], \tag{3.30}$$

where the first term on the right-hand side is the correction in the second-order terms, and the rest are the corrections to the third-order terms. Note again that the stress tensor $\boldsymbol{\sigma}$ is not a constant of motion, and must be evaluated using (3.20*c*). Evidently, ignoring terms of orders equal to or higher than τ^2, the effect of the body force acceleration $\boldsymbol{g}$ can be approximated by simply adding $\tau\boldsymbol{g}$ to the 'pre-collide' velocity $\boldsymbol{u}$.

The above procedure is rigorously defined for any orders. However, for comparison with results in existing literature (that are essentially only valid up to second order), we present in (3.31) the explicit expression of the above up to second order:

$$f_a^{(eq)} = w_a\rho\left\{1 + \boldsymbol{\xi}_a\cdot\boldsymbol{u}' + \tfrac{1}{2}\left[(\boldsymbol{\xi}_a\cdot\boldsymbol{u}')^2 - u'^2 + (\theta - 1)\left(\xi_a^2 - D\right)\right]\right.$$
$$\left. + \frac{\tau^2}{2}[(\boldsymbol{\xi}_a\cdot\boldsymbol{g})^2 + g^2]\right\}. \tag{3.31}$$

Other than the term proportional to $(\theta - 1)$, which vanishes in iso-thermal flows, and terms proportional to $\tau^2 g^2$, this is the same as the form originally proposed by Shan & Chen (1993). Furthermore, we compare the above expression to some models proposed by He, Chen & Doolen (1998*a*) and Guo, Zheng & Shi (2002) in which $f_a^{(0)}$ is given in terms of $\bar{\boldsymbol{u}} \equiv \boldsymbol{u} + \boldsymbol{g}/2$ plus an additional term linear to $\boldsymbol{g}$. Once again, it can be shown directly that they differ only by terms equal to or higher than $\boldsymbol{g}^2$. Although all these are similar in forms, there are two fundamental distinctions. First of all, the result obtained in the present formulation corresponds to a defined order of accuracy for the macroscopic moments. Clearly, the differences in (3.31) among different models can be attributed to error terms resulting in the second-order approximation. Secondly, unlike the previous approaches, the new formulation is not obtained via *a posteriori* matching for the resulting macroscopic dynamics. Furthermore, higher than the second-order approximations can be systematically and straightforwardly constructed according to the new procedure described above, which is virtually impossible via the previous approaches. More discussions on this subject are provided in the subsequent sections.

In summary (3.20) and (3.22)–(3.24) form a closed set of differential equations governing the set of variables $f_a(\boldsymbol{x}, t)$ in configuration space. The macroscopic thermohydrodynamic variables and their fluxes can be calculated directly from their corresponding moment summations. Consequently, this set of variables encompasses equivalent dynamic information about the fluid system to that represented by the thermohydrodynamic variables up to a specified moment order. The second order

($N=2$) is necessary for representing ρ, $\boldsymbol{u}$, T and the momentum flux tensor $\boldsymbol{P}$, and the macroscopic dynamics for ρ and $\boldsymbol{u}$ is described in a self-contained manner by (3.20) and (3.22)–(3.24). On the other hand, to describe the dynamics of the internal energy of a fluid system, the third-order ($N=3$) Hermite terms must be retained, as the heat flux is a component of the third moment of the distribution function. Contrary to the macroscopic thermohydrodynamic equation representations, these discrete-velocity Boltzmann equations are kinetic in nature. The form of these equations is simple and they represent an approximation to the original continuum Boltzmann equation via preserving its moments up to a specifically defined order. More importantly, higher moment order approximations to the Boltzmann equation can be systematically accomplished according to the above theoretical procedure.

4. Accuracy determination consistent with Chapman–Enskog expansion

The moment expansion procedure for the construction of the discrete Boltzmann equations is in spirit the same as that for obtaining the Grad 13-moment system. The accuracy and the range of validity in its resulting hydrodynamic behaviour are directly related to the order of truncation used in the Hermite series. Each specific truncation represents a well-defined approximation to the original Boltzmann-BGK equation. The level of accuracy is increased as higher-order terms in the truncated expansion are retained and quadratures of sufficient degree of precision employed. The necessary condition for representing the first N hydrodynamic moments has been extensively described in the previous section. On the other hand, it is important to also measure the degree of accuracy from its range in covering macroscopic physics. Here, we seek a general estimation for capturing the relevant physical effects that are associated with the level of departure from equilibrium in the Boltzmann distribution function. This estimation can be inferred through a procedure of the Chapman–Enskog expansion. As we know, the Chapman–Enskog expansion can be interpreted as an expansion in power of the Knudsen number whose value provides a measure of the degree of deviation of the Boltzmann distribution from its local equilibrium. For normal fluid flows involving slow time and large spatial scale variations, such a departure is usually small, and hence their corresponding Knudsen number values are small. Strictly speaking, the Navier–Stokes description is valid for such fluid flows only because it is derived from the Boltzmann equation by retaining terms only up to the first order in the Chapman–Enskog expansion. For fluid flows of high Knudsen number, higher-order terms in the Chapman–Enskog expansion are required to capture those no longer negligible physical effects. Unfortunately, as discussed earlier, forming closed macroscopic dynamic equations via higher-order truncations in the Chapman–Enskog expansion encounters tremendous difficulties. Obviously, owing to the kinetic level representation, we do not suffer from this kind of closure issue when going beyond the Navier–Stokes level physics. Nevertheless, the Chapman–Enskog expansion as a procedure can be useful for providing a theoretical measure in determining the order of truncation in the Hermite series for a given desired accuracy requirement. In other words, we can use the Chapman–Enskog expansion to infer a sufficient condition for the terms retained in the truncated Hermite basis that is required for describing flows of certain Knudsen number orders.

According to Chapman & Cowling (1970), we can expand f asymptotically in powers of the Knudsen number $\mathscr{K}$:

$$f=f^{(0)}+\mathscr{K}f^{(1)}+\mathscr{K}^2f^{(2)}+\cdots, \tag{4.1}$$

where at the zeroth order, $f^{(0)}$ is the equilibrium distribution of the Maxwell–Boltzmann form. Furthermore, the time and spatial variations are also measured in powers of $\mathscr{K}$, namely,

$$\partial_t = \mathscr{K}\partial_t^{(0)} + \mathscr{K}^2\partial_t^{(1)} + \cdots \tag{4.2}$$

and $\nabla = \mathscr{K}\nabla$. On substituting the above expressions into (2.7) and matching terms in the same powers of $\mathscr{K}$, we arrive at the following general recurrence relation between the distributions of order $k+1$ and those of order k and lower:

$$f^{(k+1)} = -\tau\left[\sum_{m=0}^{k}\partial_t^{(k)} f^{(m)} + \boldsymbol{\xi}\cdot\nabla f^{(k)} + \boldsymbol{g}\cdot\nabla_\xi f^{(k)}\right]. \tag{4.3}$$

Specifically, the first- and the second-order distributions, respectively, are given below,

$$f^{(1)} = -\tau\left(\partial_t^{(0)} + \boldsymbol{\xi}\cdot\nabla + \boldsymbol{g}\cdot\nabla_\xi\right) f^{(0)}, \tag{4.4a}$$

$$f^{(2)} = -\tau\left[\left(\partial_t^{(0)} + \boldsymbol{\xi}\cdot\nabla + \boldsymbol{g}\cdot\nabla_\xi\right) f^{(1)} + \partial_t^{(1)} f^{(0)}\right]. \tag{4.4b}$$

Let $\boldsymbol{a}_k^{(n)}$ be the Hermite coefficient of $f^{(k)}$, namely

$$f^{(k)} = \omega(\boldsymbol{\xi})\sum_{n=0}^{\infty}\frac{1}{n!}\boldsymbol{a}_k^{(n)}(\boldsymbol{x},t)\mathscr{H}^{(n)}(\boldsymbol{\xi}). \tag{4.5}$$

On substituting (4.5) into (4.3) and using (3.14), we obtain:

$$\boldsymbol{a}_{k+1}^{(n)} = -\tau\left[\sum_{m=0}^{k}\partial_t^{(k)}\boldsymbol{a}_{k-m}^{(n)} + \boldsymbol{\xi}\cdot\nabla\boldsymbol{a}_k^{(n)} - \boldsymbol{g}\boldsymbol{a}_k^{(n-1)}\right]. \tag{4.6}$$

Using the recurrence relation (A 4) to remove the dependence on $\boldsymbol{\xi}$ of the second term, the Hermite expansion of $f^{(k+1)}$ is obtained as the following:

$$\boldsymbol{a}_{k+1}^{(n)} = -\tau\left[\sum_{m=0}^{k}\partial_t^{(k)}\boldsymbol{a}_{k-m}^{(n)} + n\nabla\boldsymbol{a}_k^{(n-1)} + \nabla\cdot\boldsymbol{a}_k^{(n+1)} - n\boldsymbol{g}\boldsymbol{a}_k^{(n-1)}\right]. \tag{4.7}$$

We realize from (4.7) that the nth Hermite coefficients in $f^{(k+1)}$ depend only on the spatial and temporal derivatives of the Hermite coefficients in $f^{(k)}$ of orders up to $n+1$. Truncating the Hermite series of $f^{(k)}$ beyond the nth order do not affect the leading $n-1$ Hermite expansion coefficients in $f^{(k+1)}$. Consequently, if Hermite terms of order up to n are retained in the expansion of $f^{(0)}$ in (2.7), the first $n-k$ Hermite coefficients in the kth order of Chapman–Enskog expansion will be the same as if the full Maxwellian is used in (2.7). This property is extremely important as it defines a general rule that allows approximations to the Boltzmann equation at any level (measured in power of Knudsen) to be constructed by simply retaining terms at a sufficient order in the Hermite expansion and using a Gauss–Hermite quadrature of sufficient order. Moreover, this property is significant as we further notice that the momentum and energy dynamics depend on f only through its second and third moments P_{ij} and q_i, or equivalently the Hermite coefficients of up to the second and the third orders. This indicates that we must ensure the accuracy for terms up to the second or the third order in Hermite expansion. According to (4.7), the nth Hermite terms in $f^{(k)}$ depend on the accuracy of the $(n+1)$th terms in $f^{(k-1)}$, subsequently the nth hydrodynamic moment at the kth Chapman–Enskog level of approximation is satisfied if the Maxwell–Boltzmann equilibrium distribution is accurate up to $(n+k)$th order terms in Hermite expansion. For example, for the first-order (the Navier–Stokes level) Chapman–Enskog, the Maxwell–Boltzmann equilibrium distribution must be approximated in Hermite expansions to the third order in order for the pressure tensor and the momentum dynamics to be accurate at the Navier–Stokes level. It is worth noting that most LBE models (Qian *et al.* 1992; Chen & Doolen 1998) (other than a few (Chen *et al.* 1997)) correspond only to the second-order Hermite expansion. If, in addition, the heat flux and the energy dynamics must be accurate up to the Navier–Stokes level, then the fourth-order Hermite terms must be kept in the Hermite expansion of the equilibrium distribution function. More significantly, this property defines a general theoretical procedure for systematically formulating kinetic models beyond the conventional Navier–Stokes level of validity and accuracy. Specifically, by retaining up to the fourth-order terms in the Hermite expansion, we can satisfy the Burnett level accuracy pertaining to the fluid momentum evolution for isothermal systems, whereas the accuracy for the energy evolution and thermohydrodynamics is achieved at the Burnett level of accuracy if the fifth-order terms in Hermite series are retained.

In summary, we have demonstrated theoretically that the hydrodynamic behaviour of our discrete Boltzmann-BGK equation system can be made to correspond to any defined level in the Chapman–Enskog expansion, provided that sufficient terms up to a given order in (3.23) and (3.24) are retained and the quadrature formula of a sufficient degree of precision adopted. Here, the Chapman–Enskog analysis is used only to indicate a general measure of the order of accuracy as opposed to explicitly constructing macroscopic models, the resulting kinetic equation does not suffer from the closure problems encountered in the conventional representations.

5. Lattice-Boltzmann equations and extensions

In this section, we show that the commonly used LBE models are the Hermite expansions at some specific level of truncation. On the other hand, the order of accuracy is clearly determined using the new theoretical procedure. Furthermore, higher-order models can be formulated systematically. Gauss–Hermite quadratures in two- and three-dimensions are given in tables 2 and 3. The naming convention is defined in terms of three numbers as in $E_{D,n}^{d}$, where D is the dimension of the space, d the number of points (discrete velocity values) employed by the quadrature, and n the algebraic degree of precision. Comparing with the family of square and cubic lattice Boltzmann models of Qian *et al.* (1992), it is evident that the set of particle velocities in models D2Q9, D3Q15 and D3Q19 are, respectively, the abscissae in $E_{2,5}^{9}$, $E_{3,5}^{15}$ and $E_{3,5}^{19}$ scaled by a constant factor of $c=\sqrt{3}$. (In conventional LBE models, the length scale is chosen to be the lattice spacing, whereas in the discussion heretofore the length scale is chosen to be the distance that a sound wave travels in a unit of time. This difference can be trivially resolved by rescaling the length scales in our discussion by a constant c so that in the new length scale, the $\boldsymbol{\xi}_a$ corresponding to the unit lattice spacing becomes 1. In the rescaled unit, the reference sound speed becomes $1/c$.) The weights, $t_0 - t_3$, are also identical to the weights of the corresponding quadratures. The equilibrium distribution function, given in a form in which the velocities are scaled with respect to the sound speed, is exactly the second-order truncation of (3.23) with a constant unity temperature $\theta = 1$. In the hexagonal lattice Boltzmann model of Chen *et al.* (1992*a*), the set of possible particle velocities are the abscissae of $E_{2,5}^{7}$ scaled with the constant $c = 2$, in agreement with the sound speed of 1/2. On substituting the quadrature abscissae and weights into the second-order truncation of (3.23), we arrive at the following equilibrium distribution function in lattice units:

$$f_0^{(0)} = \rho(1 - 2\theta - u^2), \tag{5.1a}$$

$$f_a^{(0)} = \frac{\rho}{6}[2\theta + 2\boldsymbol{e}_a \cdot \boldsymbol{u} + 4(\boldsymbol{e}_a \cdot \boldsymbol{u})^2 - u^2] \quad (a = 1, \ldots, 6). \tag{5.1b}$$

Identifying $1 - 2\theta$ with the undetermined constant d_0 in Chen *et al.* (1992*a*), the above expressions are identical to the equilibrium distribution function therein.

In both models, only terms of up to the second order are retained in the Hermite expansion of the Maxwellian distribution to recover the momentum equation. However, according to the analysis in the previous section, the third-order terms in the Hermite expansion are required for the Navier–Stokes level of description in Chapman–Enskog expansion to survive the truncation in Hermite spectral space. The error introduced into $f^{(1)}$ by this insufficiency in expansion can be identified from (4.7) as

$$f'^{(1)} = \frac{\tau\omega}{2}\nabla \cdot \boldsymbol{a}_0^{(3)} \mathscr{H}^{(2)}. \tag{5.2}$$

Consequently, the corresponding error in the first-order Chapman–Enskog correction to the pressure tensor is:

$$P_{ij}'^{(1)} \equiv \int f'^{(1)} c_i c_j \, \mathrm{d}\boldsymbol{\xi} = \frac{\tau}{2}\nabla \cdot \boldsymbol{a}_0^{(3)} \int \omega \mathscr{H}^{(2)} c_i c_j \, \mathrm{d}\boldsymbol{\xi}, \tag{5.3}$$

where $\boldsymbol{c} = \boldsymbol{\xi} - \boldsymbol{u}$. The tensor, $c_i c_j$, can be expanded Hermite polynomials as the following:

$$\begin{aligned} c_i c_j &= \xi_i \xi_j - \xi_i u_j - \xi_j u_i + u_i u_j \\ &= \mathscr{H}_{ij}^{(2)} - u_j \mathscr{H}_i^{(1)} - u_i \mathscr{H}_j^{(1)} + (u_i u_j + \delta_{ij}) \mathscr{H}^{(0)}. \end{aligned} \tag{5.4}$$

Using the orthogonal relation, the integral in the right-hand side of (5.3) can be evaluated:

$$\int \omega \mathscr{H}_{kl}^{(2)} c_i c_j \, \mathrm{d}\boldsymbol{\xi} = \int \omega \mathscr{H}_{kl}^{(2)} \mathscr{H}_{ij}^{(2)} \, \mathrm{d}\boldsymbol{\xi} = \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}. \tag{5.5}$$

As neither model tries to simulate the energy equation, both models correspond to a constant θ. In most of the applications of these models, θ is further assumed to be unity. Hence, the error

$$P_{ij}^{(1)} \sim \tau \boldsymbol{u}^2 \nabla \cdot \boldsymbol{u} \tag{5.6}$$

is of the form of $O(Ma^3)$, which manifests as an error in viscosity of order u^2, in agreement with Qian & Orszag (1993). To avoid such an inaccuracy in the momentum equation, Hermite expansion up to the third order should be employed. The resulting equilibrium distribution function thus contains terms of the fluid velocity to the cubic power (Chen *et al.* 1997). Since, as described in the previous section, the order in Hermite expansion N requires quadrature degree $n \geqslant 2N$, an accurate Navier–Stokes level of description for an isothermal momentum equation requires a quadrature of a degree of precision greater than 6. Examples of such a quadrature are given in table 2 as $E_{2,7}^{12}$ and $E_{2,7}^{16}$ in two dimensions, and in table 3 as $E_{3,7}^{27}$ and $E_{3,7}^{33}$ in three dimensions.

It is critical to note that discrete models beyond the Navier–Stokes level of approximation can be obtained by including higher-order terms in the Hermite expansion of the Boltzmann equation and using a quadrature formula of sufficient degree. In particular, to ensure accuracy up to the Burnett order for isothermal fluids, strictly speaking we must include the Hermite expansion up to $N \geqslant 4$, and the quadrature degree up to $n \geqslant 8$. Two examples of such a quadrature are given as

$E_{2,9}^{25}$ and $E_{3,9}^{125}$, which are constructed out of $E_{1,9}^{5}$ according to the Gauss 'production' formulae as described in the Appendix. The corresponding equilibrium distribution function contains terms up to $O(u^4)$. On the other hand, for sufficiently small Mach number, the higher-order errors may be ignored. By retaining terms up to the third-order in (3.23) and (3.24), and employing a degree-7 quadrature formula such as $E_{2,7}^{12}$ and $E_{2,7}^{16}$ in two dimensions or $E_{3,7}^{27}$ and $E_{3,7}^{33}$ in three dimensions, we obtain discrete velocity models which recover the momentum equation at the Burnett level for isothermal fluids. However, for thermohydrodynamic flows, these only recover the energy equation up to the Navier–Stokes level.

It is easy to recognize that the LBE models of Qian *et al.* (1992) and Chen *et al.* (1992*a*) are formally first-order finite-difference approximations of (3.20) and (3.22)–(3.23) on special spatial grids. We discretize (3.22) in configuration space $(\boldsymbol{x}, t)$ by employing first-order upwind finite-difference approximation for the time derivative on the left-hand side:

$$\frac{\partial f_a(\boldsymbol{x},t)}{\partial t} + \boldsymbol{\xi}_a \cdot \nabla f_a(\boldsymbol{x},t) \cong \frac{1}{\Delta t}\left[f_a(\boldsymbol{x}+\boldsymbol{\xi}_a\Delta t, t+\Delta t) - f_a(\boldsymbol{x},t)\right]. \tag{5.7}$$

For convenience, we choose the time step $\Delta t = 1$, which leads to the following standard form of the Lattice Boltzmann equation:

$$f_a(\boldsymbol{x}+\boldsymbol{\xi}_a, t+1) - f_a(\boldsymbol{x},t) = -\frac{1}{\tau}\left[f_a - f_a^{(0)}\right], \tag{5.8}$$

on a spatial grid that is invariant under the transform $\boldsymbol{x} \to \boldsymbol{x} + \boldsymbol{\xi}_a$, meaning that if $\boldsymbol{x}$ is a node of the grid, $\boldsymbol{x} + \boldsymbol{\xi}_a$ are also nodes of the grid. Indeed, the quadratures $E_{2,5}^{7}$, $E_{2,5}^{9}$, $E_{3,5}^{15}$ and $E_{3,5}^{19}$ all satisfy this requirement and yield the hexagon LBGK model, and the D2Q9, D3Q15 and D3Q19 LBGK models, respectively. It is well known that such a first-order finite-difference approximation achieves second-order accuracy because of absorption of error in propagation into the effective viscosity.

The abscissae in most of the quadratures in tables 2 and 3 are not expressible as integer multiples of a common constant. For example, we can easily see that the ratios among different velocity values in $E_{3,7}^{27}$ are not rational. Models of this kind cannot be directly implemented on any simple lattices since the discrete velocities do not all coincide with the lattice nodes. The most straightforward solutions are the pointwise interpolation schemes suggested by He, Luo & Dembo (1996) or the volumetric formulation by Chen (1998). It should be pointed out that the errors introduced in the spatial discretization are non-essential, for these go to zero as spatial solution increases. This is to be differentiated from the intrinsic error in approximating the continuum Boltzmann system in discrete velocities, for the errors in the latter remain finite in spite of the spatial resolutions. Nevertheless, we should still adopt higher-order finite-difference or finite-volume schemes in order to minimize numerical diffusions when spatial resolutions are not adequate.

The quadrature formulae given in table 2 are by no means exhaustive. In higher dimensions, for a given degree of precision, finding the minimal number of points remains an active research topic. The key requirement is generally to produce the highest degree of precision with the minimal number of discrete values. This is desirable both from computational expense and accuracy considerations. However, Gaussian quadratures with discrete values made of integer multiples of a common constant are beneficial since the simple LBE form (5.8) can be realized. Besides a simple form, the simple LBE form has the advantage of ensuring an exact advection of the particle distribution function. Unlike the finite-difference (fractional advection)

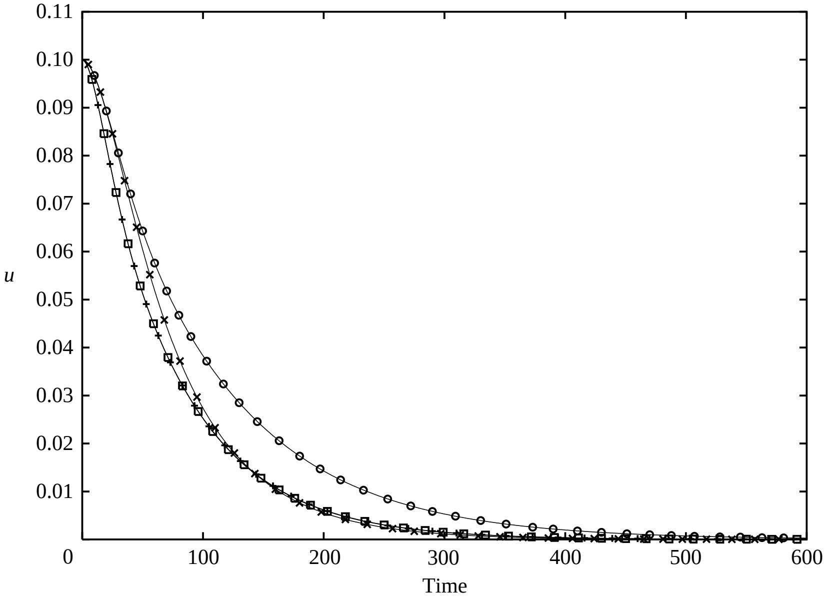

FIGURE 1. Time histories of peak velocity in shear decay simulated by the D2Q9 model and a two-dimensional projection of the 39 point model. The Knudsen number is 0.5 for all cases. ○, D3Q19; ×, D3Q19, diagonal; □, 39 point model; +, 39 point model, diagonal.

or finite-volume schemes, the simple LBE (5.8) generates zero diffusion in particle advection regardless of the distance it travels. For instance, using the non-productive formulation specified in the Appendix, $E_{3,5}^{13}$ has the same degree of precision (= 5) as $E_{3,5}^{15}$ and $E_{3,5}^{19}$, but with only 13 discrete velocity values. The price paid is, unlike $E_{3,5}^{15}$ or $E_{3,5}^{19}$, velocities in $E_{3,5}^{13}$ no longer fall on a simple lattice.

As an example to demonstrate the advantages of the new approach, simulations on the problem of transverse momentum decay at Knudsen number $\mathscr{K} \equiv 2\pi\tau c_0/L = 0.5$ were carried out in a periodic box, using both D2Q9 and a two-dimensionally projected 39-point LBM model corresponding to the quadrature $E_{3,7}^{39}$. The shear was applied along a direction either parallel or diagonal to the lattice Cartesian coordinate. Note that the decay rate in the Navier–Stokes system is determined by its shear viscosity. The existing LBM models, e.g. D3Q19 or D2Q9, can only capture such a basic feature at sufficiently small Knudsen numbers and encounter difficulties at higher Knudsen numbers. Figure 1 shows that the decay rates using D2Q9 exhibit an orientational dependency, while such a numerical artefact is completely removed in our new LBM model.

6. Discussion

In this paper, we have provided the details of a theoretical framework of LBE methods, originally proposed by Shan & He (1998). Using the Hermite expansion approach, fluid flows can be systematically approximated by constructing higher-order LBE models. Hydrodynamic moments (fluxes) at various levels can be precisely and explicitly determined at a given order of truncations. This is of central importance for the purposes of studying fluid flow at high Knudson numbers, where non-equilibrium contributions to the moments and hydrodynamic fluxes can no longer be ignored.

Compared with the standard LBE formulations, the new approach does not rely on any knowledge at the macroscopic level and does not need *a posteriori* coefficient matching, yet the agreement with macroscopic physics can be assessed order-by-order. The resulting LBE models remain in the kinetic level of representation, and retain many advantages both physically and numerically as discussed in the previous sections.

Another apparent difference is in the resulting LBE models for thermohydrodynamics. The typical forms for equilibrium distributions in standard thermal LBE has temperature θ appear in the denominators (Chen *et al.* 1997) as opposed to a constant ($\sim\theta_0$). Examining this more closely, the difference can be traced back to the scaling of microscopic velocity ξ by the temperature. It can be realized that the non-dimensionalized ξ based on a dynamical temperature encounters issues of commutating with spatial and temporal operators in the Boltzmann equation, so that the Hermite expansion procedure cannot be carried out (at least not easily). This difference has implications in terms of doing numerical simulations at higher Mach numbers. By definition, the Mach number is essentially the ratio of fluid velocity to the square root of the temperature. The standard thermal LBE can be interpreted as an expansion in terms of the local dynamic Mach number, while those from the Hermite expansions correspond to that of the characteristic Mach number. On the other hand, there is no strict requirement on the choice of value for θ_0 in principle. Hence, we may choose a higher value to ensure smaller values for the higher-order terms in the polynomial function of the equilibrium distribution.

The original Boltzmann equation was derived under the assumption of ideal gas model and the effect of intermolecular interaction was neglected. Under kinetic representation, intermolecular interaction of a fluid system can be treated by employing the mean-field approximation widely used in liquid theory (Rowlinson & Widom 1982). The effect of intermolecular interaction is approximated by an additional body force field that can then be incorporated into the kinetic equation as discussed in § 3 and by Martys *et al.* (1998). This mean-field approximation was at the centre of a previously proposed lattice Boltzmann model for non-ideal gases (Shan & Chen 1993, 1994) and has also been shown by Martys (1999) to be consistent with the classic kinetic theory for dense gases. The microscopic interaction causes a momentum exchange in the system at various locations in addition to that caused by free streaming of the particles. Of course, it is crucial that the overall momentum in the system is conserved in the absence of boundary or external influences. Regardless of the spatial scale at which the momentum of the particles is examined, be it microscopic or mesoscopic, the momentum of the particle or the collection of particles under scrutiny changes in response to the interaction. It is this additional momentum exchange that gives rise to the potential part of the pressure tensor that plays a central role in the calculation of various equilibrium properties in a phase-separated system (Rowlinson & Widom 1982). The first LBE model that is fully consistent with the above requirements was formulated over ten years ago by Shan & Chen (1993). Clearly, except for the high-order corrections, it has been shown further by He, Shan & Doolen (1998*b*) that this model can be related to the effective potential used in the Enskog theory of dense gases.

The moment expansion approach provides a better mean in the design of new discretization schemes by fully searching through the parameter spaces. The full analysis in solving the Boltzmann-BGK equation with the forcing term is our basis for further developing the discrete Boltzmann method for modelling complex fluids. The forcing term is a gateway for introducing either potential forces or other external forces into the discrete Boltzmann scheme. For multiphase fluids modelling, molecular forces specified by interaction potentials in this bottom-up approach can be readily incorporated via the forcing term of formulation presented in the previous sections. We wish to point out an important difference between the kinetic based approach for multiphase and those complex fluid models that are based on Navier–Stokes formulations by imposing some modified equations of state; even though at the equilibrium level, one may try to claim (as has been done recently) that the latter 'can' reproduce 'all' the relevant physics. Letting alone numerical simulation issues, such a claim is certainly not correct for situations where the non-equilibrium effects are significant, as is demonstrated in (3.30). Indeed, non-equilibrium effects are expected to be important at sharp interfaces as well as for high Mach- and Knudson-number flows. It is difficult (if not impossible) to capture these subtle, but important effects accurately in the existing macroscopic (hydrodynamic) representations. As a matter of principle, there is no self-consistent way macroscopically to include higher-order non-equilibrium effects in an *a priori* manner. On the contrary, a kinetic theory based ('bottom up') approach is fundamental in capturing these subtle physical properties.

Work on flow behaviour in microfluidics attracts enormous attention. As the Knudsen number increases, the Navier–Stokes equation is no longer adequate to capture the underlying fundamental physics, and its conventional higher-order corrections encounter known intrinsic difficulties. The fundamental physics is examplified by the so-called Knudsen minimum phenomenon (see Knudsen 1909; Cercignani 1975; Kang, Crone & Jhon 1999; Al-Ghoul & Eu 2004). The existing LBE models have been shown to have a certain intrinsic capability of exhibiting such an phenomenon (see Lim *et al.* 2002). Unfortunately, the discrete artefacts in these LBM are substantial enough to render the results only qualitative and suggestive at best. Certainly, the extended LBE derived from the new approach here is directly suitable for quantitative studies of such problems. Another closely related class of applications is for the air bearing problem in disk drive devices. Since the spacing for head disk interfaces is often in submicron scales, aerodynamic stability, lubrication, as well as issues of heat transfer become extremely difficult properties to understand (Fukui & Kaneko 1987; Kang *et al.* 1999). In particular, the usual no-slip boundary condition is no longer valid at finite Knudsen numbers, whereas extensive studies and modelling have been going on since the Maxwell slip model over a century ago (Maxwell 1879). We expect that the present kinetic theory based framework can offer fundamental insights into these problems, especially concerning boundary-layer formations and wetting dynamics. Moreover, the new theoretical formulation presented here allows for simulations of flows at higher-Mach-number values. Indeed, with expanded discrete velocity spaces, higher-order terms in powers of fluid velocity in the LBE equilibrium distributions can be retained. Specifically, as given in the previous sections, the maximum allowable power of the velocity terms in the distribution is a direct consequence of the order of Hermite expansions. On the contrary, most of the existing LBE models do not contain terms higher than $O(u^4)$.

Complex fluids, such as macromolecules, colloidal dispersions, bloods, mucin, synovial fluids and other functional biological fluids, exhibit a hierarchy of the characteristic length scales corresponding to the relevant microscopic structures. They usually show non-Newtonian behaviour as their characteristic relaxation times are much longer than those of simple liquids. Their dynamic processes in various length and time scales are usually strongly correlated. The small scale of microfluidics makes flow of large deformation rate easily accessible. Hence, even a low-viscosity dilute polymer solution with short relaxation time can reach a high-Deborah-number flow regime, in which elastic forces dominate over viscous forces, and so exhibit strong viscoelastic effects. Flow-induced phase separation of polymer solutions (Yuan & Jupp 2002; Jupp, Kawakatsu & Yuan 2003), can be much more pronounced. Thus progress in microfluidics gives rise to new opportunities for studying the fundamental physics of complex fluids in very strong viscoelastic flow regimes. As the dimensions of microfluidics become comparable with the intrinsic length scales of hierarchical microstructures in complex fluids, new physics start to emerge. The impact of miniaturizing fluidics on the behaviour of complex fluids is expected to be much larger and more complex. There are examples of turbulence-like instabilities (Groisman & Steinberg 2000) in the flows of polymer solutions at modest-Reynolds-number, but high-Deborah-number regimes. The present work provides a concrete theoretical basis for constructing an efficient multiple-scale computational platform for predictive modelling of such an ‘elastic turbulence’ and many other physical phenomena of complex fluids in microscopic flows.

Finally, it is straightforward to apply the Hermite moment expansion formulation to fluids involving multiple chemical species (components). Unlike the differences between isothermal and thermal flow situations, the requirement in terms of the order of accuracy for modelling multiple component fluids (including long-range interactions) is not expected to be much higher than that for the single component case. At low order, we can naturally expect recovery of the well-known scalar transport equation at the macroscopic level where the diffusion obeys Fick’s law. However, the new formulation allows us to construct LBE models at higher orders. This is useful for studying situations such as at higher Knudson-number regimes in which non-trivial scalar transport (diffusion) phenomena are to be exhibited.

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Appendix. Hermite polynomials and Gauss–Hermite quadrature

The subject of Hermite polynomials in high dimensions has been extensively treated by Grad (1949*a*). In D-dimensional Cartesian coordinates ($\boldsymbol{\xi}$), the weight function associated with the Hermite polynomials is

$$\omega(\boldsymbol{\xi}) = \frac{1}{(2\pi)^{D/2}} \exp(-\xi^2/2), \tag{A 1}$$

where $\xi^2 = \boldsymbol{\xi} \cdot \boldsymbol{\xi}$. The nth-order Hermite polynomial is defined by the Rodrigues’ formula:

$$\mathscr{H}^{(n)}(\boldsymbol{\xi}) = \frac{(-1)^n}{\omega(\boldsymbol{\xi})} \nabla^n \omega(\boldsymbol{\xi}). \tag{A 2}$$

which is an nth rank symmetric tensor and an nth degree polynomial in $\boldsymbol{\xi}$. The first few polynomials are:

$$\mathscr{H}^{(0)}(\boldsymbol{\xi}) = 1, \tag{A 3a}$$

$$\mathscr{H}^{(1)}_i(\boldsymbol{\xi}) = \xi_i, \tag{A 3b}$$

$$\mathscr{H}^{(2)}_{ij}(\boldsymbol{\xi}) = \xi_i\xi_j - \delta_{ij}, \tag{A 3c}$$

$$\mathscr{H}^{(3)}_{ijk}(\boldsymbol{\xi}) = \xi_i\xi_j\xi_k - \xi_i\delta_{jk} - \xi_j\delta_{ik} - \xi_k\delta_{ij}. \tag{A 3d}$$

The recurrence relation of Hermite polynomials is:

$$\xi_i \mathscr{H}^{(n)}(\boldsymbol{\xi}) = \mathscr{H}^{(n+1)}(\boldsymbol{\xi}) + \boldsymbol{\delta}_i \mathscr{H}^{(n-1)}(\boldsymbol{\xi}). \tag{A 4}$$

Here and throughout the manuscript, the short-hand notation of Grad (1949*a*) is adopted. A product such as the second term on the right-hand side of (A4) denotes a summation of n terms in which the second subscript of $\boldsymbol{\delta}_i$ is one of the n subscripts and $\mathscr{H}^{(n-1)}$ having the other $n-1$, that is, (A 4) is to be understood as

$$\xi_i \mathscr{H}^{(n)}_{i_1 i_2 \ldots i_n} = \mathscr{H}^{(n+1)}_{i i_1 i_2 \ldots i_n} + \sum_{k=1}^{n} \delta_{i i_k} \mathscr{H}^{(n-1)}_{i_1 i_2 \ldots i_{k-1} i_{k+1} \ldots i_n}. \tag{A 5}$$

The Hermite polynomials form a set of orthonormal bases of the Hilbert space of the functions of $\boldsymbol{\xi}$ with the inner product $\langle f, g\rangle = \int \omega f g \,\mathrm{d}\boldsymbol{\xi}$. They satisfy the following orthogonal relation:

$$\int \omega(\boldsymbol{\xi}) \mathscr{H}^{(m)}_{\boldsymbol{i}}(\boldsymbol{\xi}) \mathscr{H}^{(n)}_{\boldsymbol{j}}(\boldsymbol{\xi}) \,\mathrm{d}\boldsymbol{\xi} = \delta_{mn} \boldsymbol{\delta}^{n}_{\boldsymbol{ij}}, \tag{A 6}$$

where $\boldsymbol{i}$ is an abbreviation for the n-fold indices $i_1 i_2 \ldots i_n$; $\boldsymbol{\delta}^{n}_{\boldsymbol{ij}}$ is equal unity if the indices $(i_1, i_2, \ldots, i_n)$ are a permutation of $(j_1, j_2, \ldots, j_n)$, and zero otherwise. Any function, $f(\boldsymbol{\xi})$, that is square integrable can be expanded in terms of the Hermite polynomials as:

$$f(\boldsymbol{\xi}) = \sum_{n=0}^{\infty} \boldsymbol{a}^{(n)}_{\boldsymbol{i}} \mathscr{H}^{(n)}_{\boldsymbol{i}}(\boldsymbol{\xi}), \tag{A 7}$$

where the Einstein summation notation is understood for the n-tuple index $\boldsymbol{i}$. Multiplying by $\omega(\boldsymbol{\xi})\mathscr{H}^{(m)}_{\boldsymbol{j}}$ and integrating, we obtain:

$$\int \omega(\boldsymbol{\xi}) f(\boldsymbol{\xi}) \mathscr{H}^{(m)}_{\boldsymbol{j}}(\boldsymbol{\xi}) \,\mathrm{d}\boldsymbol{\xi} = \boldsymbol{a}^{(m)}_{\boldsymbol{i}} \boldsymbol{\delta}^{m}_{\boldsymbol{ij}} = m!\boldsymbol{a}^{(m)}_{\boldsymbol{j}}. \tag{A 8}$$

The last equality holds because there are $n!$ distinct permutations of the indices $(i_1, i_2, \ldots, i_n)$ and $\boldsymbol{a}^{(n)}_{\boldsymbol{i}}$ is fully symmetric. Alternatively, it is sometimes more convenient to use the expansion

$$f(\boldsymbol{\xi}) = \omega(\boldsymbol{\xi}) \sum_{n=0}^{\infty} \frac{1}{n!} \boldsymbol{a}^{(n)}_{\boldsymbol{i}} \mathscr{H}^{(n)}_{\boldsymbol{i}}(\boldsymbol{\xi}), \tag{A 9}$$

with the expansion coefficients given by

$$\boldsymbol{a}^{(n)}_{\boldsymbol{i}} = \int f(\boldsymbol{\xi}) \mathscr{H}^{(n)}_{\boldsymbol{i}}(\boldsymbol{\xi}) \,\mathrm{d}\boldsymbol{\xi}. \tag{A 10}$$

For a given function $f(\xi)$, Gaussian quadrature seeks to obtain the best estimate of the integral $\int_a^b \omega(\xi) f(\xi)\,\mathrm{d}\xi$ by choosing the optimal set of abscissae $\xi_a, a = 1, \ldots, n$ such that:

$$\int_a^b \omega(\xi) f(\xi) \,\mathrm{d}\xi \cong \sum_{a=1}^{n} w_a f(\xi_a), \tag{A 11}$$

where $\omega(x)$ is an arbitrary weighting function and $w_a, a = 1, \ldots, n$ a set of constant weights. The above estimate is said to have an algebraic degree of precision of m if for any f that is a polynomial of a degree up to m, exact equality holds in (A 1). The choice of ξ_a is made to maximize the algebraic degree of precision for the given number of abscissae n. The fundamental theorem of gaussian quadrature (see Krylov 1962) states that the optimal abscissae of the n-point Gaussian quadrature are

Quadrature	ξ_a	w_a
$E^1_{1,1}$	0	1
$E^2_{1,3}$	± 1	$1/2$
$E^3_{1,5}$	0	$2/3$
	$\pm\sqrt{3}$	$1/6$
$E^4_{1,7}$	$\pm\sqrt{3-\sqrt{6}}$	$(3+\sqrt{6})/12$
	$\pm\sqrt{3+\sqrt{6}}$	$(3-\sqrt{6})/12$
$E^5_{1,9}$	0	$8/15$
	$\pm\sqrt{5-\sqrt{10}}$	$(7+2\sqrt{10})/60$
	$\pm\sqrt{5+\sqrt{10}}$	$(7-2\sqrt{10})/60$

TABLE 1. One-dimensional Gauss–Hermite quadrature formulae. $\boldsymbol{\xi}$ are the abscissae and w the weights. A quadrature formula is named by three numbers as in $E^d_{D,n}$, where D is the dimension of the space, n the algebraic degree of precision, and d the number of points employed by the quadrature. In one dimension, the algebraic degree of precision is $2n-1$, where n is the number of abscissae used in the quadrature.

precisely the roots of the nth corresponding orthogonal polynomial, and the weights are given by:

$$w_a = \frac{\langle P_{n-1}, P_{n-1}\rangle}{P_{n-1}(\xi_a)P_n'(\xi_a)}, \tag{A 12}$$

where $P_n' = \mathrm{d}P_n/\mathrm{d}x$. Equation (A 11) has an algebraic degree of precision of $2n-1$.

In one dimension, the Gauss–Hermite quadrature is the Gauss quadrature over the interval $(-\infty, \infty)$ with respect to the weight function of (A 11). The corresponding orthogonal polynomials are the Hermite polynomials and the abscissae of the n-point quadrature are the zeros of $\mathscr{H}^{(n)}$. Taking the derivative of (A 2), we obtain

$$\frac{\mathrm{d}\mathscr{H}^{(n)}}{\mathrm{d}\xi} = \xi\mathscr{H}^{(n)} - \mathscr{H}^{(n+1)} = n\mathscr{H}^{(n-1)}. \tag{A 13}$$

Using (A 4) and (A 6), the corresponding weights are:

$$w_a = \frac{n!}{[n\mathscr{H}^{(n-1)}(\xi_a)]^2}. \tag{A 14}$$

Table 1 gives the numerical values of the abscissae and weights of Gauss–Hermite quadratures up to $n=5$, degree-9. For convenience, we shall hereinafter name the quadrature formulae by the convention $E^d_{D,m}$ where D is the dimension of the space, m ($=2n-1$ in one dimension) is the algebraic degree of precision, and d ($=n$ in one dimension) is the number of points employed in the quadrature. For example, $E^9_{2,5}$ denotes a degree-5 quadrature formula in two dimensions employing 9 points.

In higher dimensions, no general Gauss quadrature theory is known. Nevertheless, a class of Gauss–Hermite formulae known as 'production' formulae can be derived form one-dimensional formulae. Consider the following type of multiple integrals:

$$\frac{1}{(2\pi)^{D/2}}\int \exp(-\xi^2/2)p(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi} \tag{A 15}$$

where $p(\boldsymbol{\xi})$ is a D-dimensional polynomial of degree n of the following general form:

$$p(\boldsymbol{\xi}) = \sum_{n_1+\cdots+n_D \leqslant n} a_{n_1 n_2 \cdots n_D} \prod_{j=1}^{D} \xi_j^{n_j}. \tag{A 16}$$

We notice that for each individual term, the integration is separable and an approximation to the integral can be obtained by applying the one-dimensional formula repeatedly. Let w_a and ξ_a, $a = 1, \ldots, n$, be the weights and abscissae of a one-dimensional degree-n quadrature formula, for each term in the equation above, we can write:

$$\begin{aligned}\frac{1}{(2\pi)^{D/2}} \int \exp(-\xi^2/2) \prod_{j=1}^{D} \xi_j^{n_j}\, \mathrm{d}\boldsymbol{\xi} &= \prod_{j=1}^{D} \left(\frac{1}{\sqrt{2\pi}} \int \exp(-\xi_j^2/2) \xi_j^{n_j}\, \mathrm{d}\xi_j \right) \\ &= \prod_{j=1}^{D} \left(\sum_{a=1}^{n} w_a \xi_a^{n_j} \right) = \sum_{k_1=1}^{n} \cdots \sum_{k_D=1}^{n} w_{k_1} \cdots w_{k_D} \xi_{k_1}^{n_1} \cdots \xi_{k_D}^{n_D},\end{aligned} \tag{A 17}$$

where the second equality holds because $n_j \leqslant n$ for all j. If we define the D-dimensional abscissae as the vectors $\boldsymbol{\xi}_{k_1 \cdots k_D} = (\xi_{k_1}, \xi_{k_2}, \ldots, \xi_{k_D})$, and the corresponding weights as $w_{k_1 \cdots k_D} = w_{k_1} w_{k_2} \cdots w_{k_D}$, $k_i = 1, \ldots, d$ for $i = 1, \ldots, D$ – there are a total of d^D pairs of them – and multiply (A 17) by the coefficient $a_{n_1 \cdots n_D}$ and sum over all terms, we obtain the following D-dimensional Gauss–Hermite quadrature formula based on the one-dimensional formula:

$$\frac{1}{(2\pi)^{D/2}} \int \exp(-x^2/2) p(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x} = \sum w_{k_1 \cdots k_D} p(\boldsymbol{\xi}_{k_1 \cdots k_D}). \tag{A 18}$$

Particularly, applying the one-dimensional formula $E_{1,5}^{3}$ in two- and three-dimensions yields $E_{2,5}^{9}$ and $E_{3,5}^{27}$ in table 2, both of degree 5.

For the case of degree-5 quadrature in three dimensions, the production formula $E_{3,5}^{27}$ employs all the 27 Cartesian grid points. By examining (A 17), quadrature formulae that do not require all the 27 points can be obtained. We denote the weight of the abscissa $(0, 0, 0)$ by $w_{(0,0,0)}$, that of the abscissa $(0, 0, \sqrt{3})$ by $w_{(0,0,1)}$ and so on. Because of symmetry requirements, the weights of the abscissae belonging to the same symmetry group must equal each other, e.g. $w_{(0,0,1)} = w_{(0,0,-1)} = w_{(0,1,0)}$ etc. Without loss of generality, we let $n_1 \leqslant n_2 \leqslant n_3$. Obviously, $n_1 \leqslant 1$, since $n_i \geqslant 0$ for $i = 1, 2, 3$ and $n_1 + n_2 + n_3 \leqslant 5$. At $n_1 = 1$, the integral is always zero because the integrand is antisymmetric with respect to the plane $\xi_1 = 0$. As long as the weights are symmetric with respect to the plane $\xi_1 = 0$, the sum on the right-hand side of (A 17) is zero and the quadrature is exact. In the case of $n_1 = 0$, where the integrand is a two-dimensional function, the quadrature is exact if and only if the weights reduce to that of $E_{2,5}^{9}$ by satisfying the following relation:

$$w_{(0,0,0)} + 2w_{(0,0,1)} = 4/9, \tag{A 19a}$$

$$w_{(0,0,1)} + 2w_{(0,1,1)} = 1/9, \tag{A 19b}$$

$$w_{(0,1,1)} + 2w_{(1,1,1)} = 1/36, \tag{A 19c}$$

where on the right-hand side are the weights of $E_{2,5}^{9}$. Noticing that there is one fewer equation than the number of variables, the general solution is given by the parametric

Quadrature	$\boldsymbol{\xi}_a$	Group	p	w_a	
$E_{2,4}^{6}$	$(0,0)$	A	1	$1/2$	
	$2\left(\cos\frac{2n\pi}{5},\sin\frac{2n\pi}{5}\right)$	B	5	$1/10$	$n=1,\ldots,5$
$E_{2,5}^{7}$	$(0,0)$	A	1	$1/2$	
	$2\left(\cos\frac{n\pi}{3},\sin\frac{n\pi}{3}\right)$	B	6	$1/12$	$n=1,\ldots,6$
$E_{2,5}^{9}$	$(0,0)$	A	1	$4/9$	
	$(\sqrt{3},0)_{FS}$	B	4	$1/9$	
	$(\pm\sqrt{3},\pm\sqrt{3})$	C	4	$1/36$	
$E_{2,7}^{12}$	$(r,0)_{FS}$	A	4	$1/36$	$r^2=6$
	$(\pm s,\pm s)$	B	4	$(5+2\sqrt{5})/45$	$s^2=(9-3\sqrt{5})/4$
	$(\pm t,\pm t)$	C	4	$(5-2\sqrt{5})/45$	$t^2=(9+3\sqrt{5})/4$
$E_{2,7}^{16}$	$(r,0)_{FS}$	A	4	$(5-2\sqrt{6})/48$	$r^2=3+\sqrt{6}$
	$(s,0)_{FS}$	B	4	$(5+2\sqrt{6})/48$	$s^2=3-\sqrt{6}$
	$(r,s)_{FS}$	C	8	$1/48$	
$E_{2,7}^{17}$	$(0,0)$	A	1	$(575+193\sqrt{193})/8100$	
	$(r,0)_{FS}$	B	4	$(3355-91\sqrt{193})/18\,000$	$r^2=(125+5\sqrt{193})/72$
	$(\pm r,\pm r)$	C	4	$(655+17\sqrt{193})/27\,000$	
	$(\pm 2r,\pm 2r)$	E	4	$(685-49\sqrt{193})/54\,000$	
	$(3r,0)_{FS}$	D	4	$(1445-101\sqrt{193})/162\,000$	

TABLE 2. Gauss–Hermite quadrature formulae in two dimensions. Here, p is the number of abscissae in the symmetry class. The subscript $_{FS}$ denotes a fully symmetric set of points. The abscissae of quadrature $E_{2,4}^{6}$ correspond to the vertices of a pentagon. The abscissae of quadrature $E_{2,5}^{7}$ correspond to the vertices of a hexagon. $E_{2,5}^{9}$ is a 'production' formula of $E_{1,5}^{3}$ in two dimensions. $E_{2,7}^{12}$ and $E_{2,7}^{16}$ are due to Stroud (1971) and their abscissae are depicted in figure 2. $E_{2,7}^{17}$ is obtained by solving (A 25) on a Cartesian grid.

equation:

$$\begin{pmatrix} w_{(0,0,0)} \\ w_{(0,0,1)} \\ w_{(0,1,1)} \\ w_{(1,1,1)} \end{pmatrix} = \frac{1}{72}\begin{pmatrix} 8(2-t) \\ 4(t-2) \\ 2t \\ 1-t \end{pmatrix}. \tag{A 20}$$

At $t=0$ and 1, we obtain formulae $E_{3,5}^{15}$ and $E_{3,5}^{19}$ using 15 and 19 of the grid points, respectively. In addition, $E_{3,5}^{27}$ corresponds to the special case of $t=2/3$.

Non-production quadrature formulae requiring fewer points can be obtained using other methods. A comprehensive list of quadrature formulae for the integral $\int\exp(-\xi^2)f(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi}$ is given by Stroud (1971). They can be easily converted for use with the weight function (A 1). Let $\boldsymbol{\xi}_i'$ and w_i' be the abscissae and weights for the integral $\int\exp(-\xi^2)f(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi}$, namely,

$$\int\exp(-\xi^2)f(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi} = \sum w_a' f(\boldsymbol{\xi}_a'). \tag{A 21}$$

After the transforms $\boldsymbol{\xi}=\boldsymbol{\zeta}/\sqrt{2}$ and $f(\boldsymbol{\xi})=g(\sqrt{2}\boldsymbol{\xi})$ and multiplying by $\pi^{-D/2}$, we have

$$\frac{1}{(2\pi)^{D/2}}\int\exp(-\zeta^2/2)g(\boldsymbol{\zeta})\,\mathrm{d}\boldsymbol{\zeta} = \sum\frac{w_a'}{\pi^{D/2}}g(\sqrt{2}\boldsymbol{\xi}_a'). \tag{A 22}$$

Quadrature	$\boldsymbol{\xi}_a$	Group	p	w_a	
$E_{3,5}^{13}$	$(0,0,0)$	A	1	$2/5$	
	$(\pm r, \pm s, 0)$	B	4	$1/20$	$r^2=(5+\sqrt{5})/2$
	$(0, \pm r, \pm s)$	B	4	$1/20$	$s^2=(5-\sqrt{5})/2$
	$(\pm s, 0, \pm r)$	B	4	$1/20$	
$E_{3,5}^{15}$	$(0,0,0)$	A	1	$2/9$	
	$(\sqrt{3},0,0)_{FS}$	B	6	$1/9$	
	$(\pm\sqrt{3}, \pm\sqrt{3}, \pm\sqrt{3})$	C	8	$1/72$	
$E_{3,5}^{19}$	$(0,0,0)$	A	1	$1/3$	
	$(\sqrt{3},0,0)_{FS}$	B	6	$1/18$	
	$(\sqrt{3},\sqrt{3},0)_{FS}$	C	12	$1/36$	
$E_{3,5}^{27}$	$(0,0,0)$	A	1	$8/27$	
	$(\sqrt{3},0,0)_{FS}$	B	6	$2/27$	
	$(\sqrt{3},\sqrt{3},0)_{FS}$	C	12	$1/54$	
	$(\pm\sqrt{3}, \pm\sqrt{3}, \pm\sqrt{3})$	D	8	$1/216$	
$E_{3,7}^{27}$	$(0,0,0)$	A	1	$(720 \pm 8\sqrt{15})/2205$	
	$(r,0,0)_{FS}$	B	6	$(270 \mp 46\sqrt{15})/15435$	$r^2=(15\pm\sqrt{15})/2$
	$(s,s,0)_{FS}$	C	12	$(162 \pm 41\sqrt{15})/6174$	$s^2=6\mp\sqrt{15}$
	$(\pm t, \pm t, \pm t)$	D	8	$(783 \mp 202\sqrt{15})/24696$	$t^2=9\pm\sqrt{15}$
	Two formulae, use either upper or lower sign.				
$E_{3,7}^{39}$	$(0,0,0)$	A	1	$1/12$	
	$(r,0,0)_{FS}$	B	6	$1/12$	$r^2=3/2$
	$(\pm r, \pm r, \pm r)$	C	8	$1/27$	
	$(2r,0,0)_{FS}$	D	6	$2/135$	
	$(2r,2r,0)_{FS}$	E	12	$1/432$	
	$(3r,0,0)_{FS}$	F	6	$1/1620$	

TABLE 3. Gauss–Hermite quadrature formulae in three dimensions. $E_{3,5}^{13}$ is the minimum degree-5 quadrature known in three dimensions. Its abscissae correspond to the vertices of a icosahedron. $E_{3,5}^{15}$, $E_{3,5}^{19}$ and $E_{3,5}^{27}$ are 'production' formulae of $E_{1,5}^{3}$ in three dimensions. They correspond to the D3Q15, D3Q19 and D3Q27 LBGK models. Qian *et al.* (1992) respectively. $E_{3,7}^{27}$ is due to Stroud (1971). $E_{3,7}^{39}$ is obtained by solving (A 25) on a Cartesian grid.

Therefore, for the type of integrals in (A 15), the abscissae and weights are $\boldsymbol{\xi}_a = \sqrt{2}\boldsymbol{\xi}'_a$ and $w_a = w'_a/\pi^{D/2}$. Some of the quadratures in table 2 are adopted from Stroud (1971). Of particular interests are $E_{2,5}^{7}$ and $E_{3,5}^{13}$ which are the known degree-5 formulae with the smallest number of points in two- and three-dimensions, respectively. Quadratures $E_{2,7}^{12}$ and $E_{2,7}^{16}$ are also adopted from Stroud (1971). Figure. 2 shows the abscissae of these two quadratures.

Except for a few special cases, the abscissae of the Gauss–Hermite quadratures discussed so far generally do not coincide with normal Cartesian coordinates. Sometimes it is highly desirable to have quadratures with abscissae being the grid points of Cartesian coordinates. It is worth pointing out that quadratures on predefined abscissae can be constructed by explicitly solving (A 11) with f being a polynomial of degree m. Let $\{P_i(\xi), i=0,\ldots,\infty\}$ be the set of orthonormal polynomials on the interval $[a,b]$ with respect to the weight function $\omega(\xi)$, which is

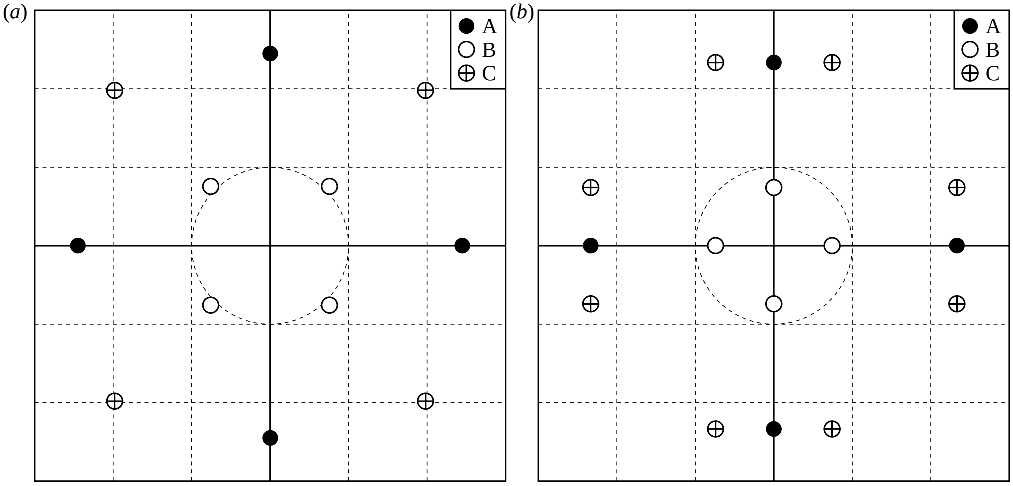

FIGURE 2. Abscissae of two degree-7 Gauss–Hermite quadrature formulae in two–dimensions: (*a*) $E^{12}_{2,7}$ and (*b*) $E^{16}_{2,7}$. The unit circle in the middle depicts the sound speed. The type of symbols denotes the symmetry group that an abscissa belongs to (cf. table 2).

normalized so that $\int_a^b \omega \,\mathrm{d}\xi = 1$. It follows the orthonormal relation that $P_0 = 1$, and

$$\int_a^b \omega(x) P_i(\xi)\,\mathrm{d}\xi = \begin{cases} 1, & i = 0, \\ 0, & i \neq 0. \end{cases} \tag{A 23}$$

Since $\{P_i, i = 0, \ldots, \infty\}$ is a complete set of expansion bases, f can be expanded as

$$f(\xi) = \sum_{i=0}^{m} a_i P_i(\xi), \tag{A 24}$$

where a_i are the expansion coefficients. Obviously, (A 11) is exact if and only if w_a and ξ_a satisfy the following equations:

$$\sum_{a=1}^{d} w_a P_i(\xi_a) = \begin{cases} 1, & i = 0, \\ 0, & i = 1, \ldots, m. \end{cases} \tag{A 25}$$

For a given set of abscissae, solutions to the above equations generally exist as long as a sufficient number of abscissae are used. Of course, the number of abscissae is greater than the number of abscissae in the optimal Gauss quadratures which are obtained when the abscissae are allowed to change. On substituting the multi-dimensional Hermite polynomials into (A 25), and choosing the abscissae as the grid points of Cartesian coordinates (up to a constant scaling factor), we obtain two degree-7 quadratures, $E^{17}_{2,7}$ and $E^{39}_{3,7}$.

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