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On-node lattices construction using partial Gauss–Hermite quadrature for the lattice Boltzmann method*

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A concise theoretical framework, the partial Gauss–Hermite quadrature (pGHQ), is established to construct on-node lattices of the lattice Boltzmann (LB) method under a Cartesian coordinate system. Compared with the existing approaches, the pGHQ scheme has the following advantages: extremely concise algorithm, unifies the constructing procedure for symmetric and asymmetric on-node lattices, and covers a full-range quadrature degree of a given discrete velocity set. We employ the pGHQ scheme to search the local optimal and asymmetric lattices for $\{n=3,4,5,6,7\}$ moment degree equilibrium distribution discretization on the range $[-10,10]$. The search reveals a surprising abundance of available lattices. Through a brief analysis, the discrete velocity set shows a significant influence on the positivity of equilibrium distributions, which is considered as one of the major impacts of the numerical stability of the LB method. Hence, the results of the pGHQ scheme lay a foundation for further investigations to improve the numerical stability of the LB method by modifying the discrete velocity set. It is also worth noting that pGHQ can be extended into the entropic LB model, even though it was proposed for the Hermite polynomial expansion LB theory.

Keywords: equilibrium distribution discretization, partial Gauss–Hermite quadrature

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1. Introduction

The lattice Boltzmann (LB) method is a powerful approach for hydrodynamics.[1,2] The essence of the LB method is an intuitively parallel collision-streaming algorithm with discretized position $\boldsymbol{r}$, time t, and microscopic velocity $\boldsymbol{v}_\alpha$

$$f_\alpha(\boldsymbol{r}+\boldsymbol{v}_\alpha\delta_t,t+\delta_t)=\left(1-\frac{1}{\tau}\right)f_\alpha(\boldsymbol{r},t)+\frac{1}{\tau}f_\alpha^{\rm eq}(\boldsymbol{r},t), \quad (1)$$

where f_α and $f_\alpha^{\rm eq}$ are, respectively, the population and equilibrium distribution corresponding to the discrete velocity $\boldsymbol{v}_\alpha$. Equation (1) can be treated as a characteristic integral of the Bhatnagar–Gross–Krook (BGK)–Boltzmann equation along $\boldsymbol{v}_\alpha$,[3,4] depicting the microscopic dynamic of particles. With specific discretization of the continuous BGK–Boltzmann equation in velocity space (i.e., on-node lattices), each collision-streaming proceeding would locate on nodes, achieving a simple but efficient "stream along links and collide at nodes" algorithm, while the corresponding macroscopic dynamics such as the Navier–Stokes equations can be properly recovered. In practice, this velocity discretization can be achieved by constructing a set of equilibrium distributions $\{f_\alpha^{\rm eq}\}$ on a discrete velocity set $\{v_\alpha\}$; i.e., equilibrium distribution (ED) discretization. Under a Cartesian coordinate system, multidimensional $f_\alpha^{\rm eq}$ can always be constructed as a tensor product of the unidimensional $f_\alpha^{\rm eq}$. This enables us to focus on the unidimensional Cartesian model to simplify our framework.

The ED discretization has been investigated in-depth and a lot of excellent theories have been proposed, such as the small-Mach-number approximation,[5] the Hermite polynomial expansion,[6] and the entropic LB model.[7] According to the Hermite polynomial expansion,[6,8,9] for nth-moment-order ED discretization which restores u^n moment integral, its $f_\alpha^{\rm eq}$ can be expressed as

$$f_\alpha^{\rm eq}=w_\alpha\rho\sum_{i=0}^{n}H_i(\xi_\alpha)\frac{\phi^i}{i!}, \quad (2)$$

where

$$\rho=\sum_{\alpha=0}^{q-1}f_\alpha^{\rm eq}, \quad \phi=\sum_{\alpha=0}^{q-1}f_\alpha^{\rm eq}\xi_\alpha/\rho, \quad (3)$$

$$w_\alpha=\frac{1}{\sqrt{\pi}}\int {\rm e}^{-\xi^2}\prod_{\substack{\beta=0\\ \beta\neq\alpha}}^{q-1}\frac{\xi-\xi_\beta}{\xi_\alpha-\xi_\beta}{\rm d}\xi. \quad (4)$$

Here, $\xi=v/\sqrt{2RT}$ and $\phi=u/\sqrt{2RT}$ are the dimensionless variables of microscopic velocity v and macroscopic velocity u, respectively, in which R is the gas constant and T is the temperature. $H_i(\xi)$ is the ith Hermite polynomial, and $\{\xi_0,\ldots,\xi_{q-1}\}$ is the corresponding discrete set (or abscissas) which evaluates the integral exactly for $k\leq 2n$

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$$I^k = \int \frac{1}{\sqrt{\pi}} \mathrm{e}^{-\xi^2} \xi^k \mathrm{d}\xi = \sum_{\alpha=0}^{q-1} w_\alpha \xi_\alpha^k. \tag{5}$$

The abscissas and the discrete velocity set have the relation $\xi_\alpha = v_\alpha/\sqrt{2RT}$. The Hermite polynomial expansion converts the nth-moment-order ED discretization under a unidimensional Cartesian coordinate system into a pure $2n$-degree quadrature problem; i.e., constructing the smallest abscissas $\{\xi_0, \ldots, \xi_{q-1}\}$ fulfilling Eq. (5) for all $k \leq 2n$. One can refer to Section 1 in the Supplementary Material for the detail derivation. For the sake of simplifying the discussion, we designate Eq. (5) as quadrature equation (QE) and its equation system of all $k \leq n$ as nth quadrature equation system (QES). It should be noted that the nth QES is the detail governing equation system for a given abscissa set $\{\xi_\alpha\}$ with quadrature degree n. Hence, in the discussion hereinafter, QES and quadrature degree shall be used indistinguishably.

An available smallest quadrature for $2n$th QES is the $(n+1)$th Gauss–Hermite quadrature, which are the zeros of $(n+1)$th Hermite polynomial. The issue is that the zeros of an Hermite polynomial with degree above 3 cannot fit into nodes, which means that they cannot be expressed as $\{v_0, \ldots, v_{q-1}\}c$, where v and c stand for integer-valued discrete micro velocity and real-valued lattice constant $1/\sqrt{2RT}$, respectively. This leads to an off-node lattices in $u^{n\geq 3}$ ED discretization. Hence, to construct an on-node lattices for $u^{n\geq 3}$ ED discretization—i.e., $\{v_0, \ldots, v_{q-1}\}c$-type quadrature—one has to manually solve QES, which involves both $\{\xi_\alpha\}$ and $\{w_\alpha\}$. To simplify the notation, in the discussion hereinafter, "lattices" would directly denote "on-node lattices" unless otherwise stated. In practice, a symmetric discrete velocity set $\{0, \pm v_1, \ldots, \pm v_m\}$ is predefined. This avoids the computation of QE with odd exponent k, which significantly simplifies QES, and makes QES purely consist of c and $\{w_\alpha\}$. Employing the skills in Refs. [9] and [10] to deal with QES, a univariate polynomial equation for lattice constant c can be obtained, which separates the co-solving of c and $\{w_\alpha\}$. This leads us to a performable construction of on-node lattices. Actually, this univariate polynomial equation can be directly obtained through a mathematical tool and avoids the tedious QES solving.

In this paper, the partial Gauss–Hermite quadrature (pGHQ) mathematical tool is proposed. The pGHQ is a quadrature rule derived from the Gauss–Hermite quadrature. It keeps the most desirable characteristic of the Gauss–Hermite quadratur; i.e., its quadrature is constructed directly on abscissa polynomial avoiding the co-solving of $\{\xi_\alpha\}$ and $\{w_\alpha\}$ in QES. Meanwhile, it offers a performable approach for on-node lattices construction. The on-node lattices construction in the pGHQ scheme is extremely concise. Once a discrete velocity set has been given, a full-range univariate polynomial equation system of its lattice constant c would be directly obtained through pGHQ. Compared with the existing schemes, our approach has the following advantages: (i) the algorithm is extremely concise; (ii) the procedure to construct the univariate polynomial equations is unified for both symmetric and asymmetric lattices; and (iii) the generated univariate polynomial equation system covers full-range quadrature degree of the given $\{v_0, \ldots, v_{q-1}\}$. We will elaborate these points in detail in the following.

2. pGHQ theory and implementation

The theory of pGHQ can be stated as follows: for a q-point abscissa set $\{\xi_\alpha\}$, whose abscissa polynomial $W_q(\xi) = \prod_{\alpha=0}^{q-1}(\xi - \xi_\alpha)$ satisfies the orthogonal relationship

$$\int \mathrm{e}^{-\xi^2} W_q(\xi)\, p(\xi)\, \mathrm{d}\xi = 0, \quad \forall p(\xi) \in \mathbb{P}_{K(K<q)}, \tag{6}$$

where $\mathbb{P}_K$ is the set of polynomials of degrees not exceed K, it has $(q+K)$ quadrature degree indicating that the set $\{\xi_\alpha\}$ and its corresponding $\{w_\alpha\}$ calculated by Eq. (4) fulfill $(q+K)$th QES . The pGHQ is a generalization of the Gauss–Hermite quadrature, which is the special case of Eq. (6) with polynomial degree $K = (q-1)$. Given any polynomial $p(\xi)$ of degree not exceeding K, it can always be expressed as a linear combination of Hermite polynomials with degree not exceeding K

$$p(\xi) = \sum_{i=0}^{K} c_i \xi^i = \sum_{i=0}^{K} a_i H_i(\xi). \tag{7}$$

Employing the orthogonal relationship of Hermite polynomials

$$\int \mathrm{e}^{-\xi^2} H_i(\xi) H_j(\xi)\, \mathrm{d}\xi = \begin{cases} 0, & i \neq j, \\ 2^i i! \sqrt{\pi}, & i = j, \end{cases} \tag{8}$$

the orthogonality in Eq. (6) indicates that for a q-point quadrature with $q+K$ quadrature degree, its abscissa polynomial does not involve Hermite polynomials with degree below $K+1$ when written in the Hermite polynomial form; i.e., all the coefficients of Hermite polynomials with degree below $K+1$ are zero

$$W_q(\xi) = \sum_{i=0}^{q} A_i H_i(\xi) = \sum_{i=K+1}^{q-1} A_i H_i(\xi) + \frac{1}{2^q} H_q(\xi). \tag{9}$$

Because A_i is an expression of the abscissas $\{\xi_\alpha\}$, then the zero coefficients $\{A_i = 0 | i \leq K\}$ could be used as the governing equation system of the abscissas under pGHQ for $q+K$ quadrature degree. For the detail derivation, one can refer to Section 2 in the Supplementary Material. Hence, for a q-point set $\{\xi_\alpha\}$, once the coefficient equations $\{A_i = 0\}$ are satisfied for all $i \leq K$ in its Hermite-polynomial-form abscissa polynomial Eq. (9), this set and its corresponding $\{w_\alpha\}$ in Eq. (4) fulfill $(q+K)$th QES. This coefficient equation system is denoted as Hermite coefficient equation system (HCES) in this paper. To identify an HCES, the denotation $q \sim K^{\text{th}}$ is added before HCES, in which q is the abscissa number, K denotes the equations contained in the HCES $\{A_i = 0 | i \leq K\}$, and $(q+K)$

is its corresponding quadrature degree. HCES is equivalent to QES but without involving $\{w_\alpha\}$. It indicates that pGHQ owns the desirable characteristic of the Gauss–Hermite quadrature, constructing the quadrature directly on abscissa polynomial avoiding the co-solving of $\{\xi_\alpha\}$ and $\{w_\alpha\}$ in QES.

Now, we employ pGHQ to construct the univariate polynomial equation of c. The univariate polynomial equation of c essentially is a relation between c and the quadrature degree of the corresponding abscissa set $\{v_0,\ldots,v_{q-1}\}c$. Once the equation is satisfied, its corresponding $\{v_0,\ldots,v_{q-1}\}c$ possesses a certain quadrature degree, fulfilling QES with a specific order. In classical approaches,[8,10] it is obtained through manually computing the QES, which needs to construct the QES and separate the co-solving of c and $\{w_\alpha\}$. Now, as the previous discussion shows that HCES is an equation system equivalent to QES but without involving $\{w_\alpha\}$, this relation can be directly constructed by calculating its Hermite polynomial coefficients $\{A_i\}$ in abscissa polynomial. Given a predefined $\{v_0,\ldots,v_{q-1}\}$ with an unknown lattice constant c, we substitute it into the abscissa polynomial with relation $\xi_\alpha = v_\alpha c$, and expand the product

$$W_q(\xi) = \prod_{\alpha=0}^{q-1}(\xi - v_\alpha c) = \sum_{k=0}^{q} b_k \xi^k, \tag{10}$$

where b_k is a univariate polynomial of c. Introducing the explicit expressions for monomial in terms of Hermite polynomials

$$\xi^k = \frac{k!}{2^k}\sum_{l=0}^{\lfloor k/2\rfloor}\frac{1}{l!\,(k-2l)!}H_{k-2l}(\xi), \tag{11}$$

where $\lfloor\cdot\rfloor$ is the floor function, equation (10) can be converted into Hermite polynomial form

$$W_q(\xi) = \sum_{i=0}^{q} A_i H_i(\xi). \tag{12}$$

Since equation (11) does not involve new unknown variables, coefficient A_i is still a univariate polynomial of c. According to the pGHQ theory, a series of $q \sim K^{\text{th}}$ HCES could be constructed for $\{v_0,\ldots,v_{q-1}\}c$, where $0 \le K \le q-1$. They cover all possible quadrature degrees of the discrete velocity set, from q to $2q-1$. These series of HCES are the target univariate polynomial equation systems of c, which in classical approaches are constructed through solving QES. Hence, the on-node lattices construction in the pGHQ scheme is simply performed on the abscissa polynomial without calculating QES and separating the co-solving of lattice constant c and weights $\{w_\alpha\}$. Taking $\{0,\pm1,\pm5\}$ as an example, after converting its abscissa polynomial into the Hermite polynomial form

$$W_q(\xi) = \prod_{\alpha=0}^{4}(\xi - v_\alpha c) = \xi^5 - 26c^2\xi^3 + 25c^4\xi^1 = \sum_{i=0}^{5} A_i H_i(\xi), \tag{13}$$

where the coefficients $\{A_i\}$ read

$$A_5 = \frac{1}{32},\quad A_4 = 0,\quad A_3 = \frac{5}{8} - \frac{26c^2}{8},\quad A_2 = 0,$$
$$A_1 = \frac{15}{8} - \frac{78c^2}{4} + \frac{25c^4}{2},\quad A_0 = 0, \tag{14}$$

its series of HCES could be directly generated. For an instance, its $5 \sim 4^{\text{th}}$ HCES $\{A_i = 0 | i \le 4\}$ is

$$0 = 0,\quad \frac{15}{8} - \frac{78c^2}{4} + \frac{25c^4}{2} = 0,$$
$$0 = 0,\quad \frac{5}{8} - \frac{26c^2}{8} = 0,\quad 0 = 0. \tag{15}$$

Once this HCES has real-valued solution c, $\{0,\pm1,\pm5\}c$ satisfies the 9th QES. It is worth noting that the $\{0,\pm1,\pm5\}c$ corresponding to Eq. (15) is the 5th Gauss–Hermite quadrature, which as mentioned before is off-node. This off-node characteristic is reflected as no real solution c for its HCES. Equation (14) presents the most significant advantage of the pGHQ scheme; i.e., comparing with the generation of a specific univariate polynomial equation in classical approaches,[8,10] the pGHQ scheme systematically offers a series of HCES for lattice constant c once the expressions of coefficients $\{A_i\}$ are obtained.

In practice, given a discrete velocity set $\{v_0,\ldots,v_{q-1}\}$, the quadrature degree of $\{v_0,\ldots,v_{q-1}\}c$ is required to be as high as possible so that it can be used to construct higher moment degree ED discretization. Therefore, one can start with solving its $q \sim (q-1)^{\text{th}}$ HCES, where $K = q-1$ is theoretically the largest. Once this HCES has no real-valued solutions for c, one decreases K by 1. As the construction of HCES shows, this decreasing is actually loosing the constraints on lattice constant c by reducing the governing equations $\{A_i = 0\}$. This procedure is repeated until a real-valued c is found. Its corresponding K gives the quadrature degree of $\{v_0,\ldots,v_{q-1}\}c$, $q+K$, which indicates that this set can be used to construct the $u^{\lfloor (q+K)/2\rfloor}$ ED discretization. The construction of f_α^{eq} is illustrated in Eq. (2). We designate this approach as the pGHQ scheme. It should be noted that there is no limitation on the given discrete velocity set. Given any kind of discrete velocity set, whether it is symmetric or asymmetric, the coefficients $\{A_i\}$ can always be obtained and their procedures are unified with the same formulas Eqs. (10)–(12), which is another great advantage of the pGHQ scheme. Hence, the pGHQ scheme supports constructing all kinds of lattices, symmetric or asymmetric.

Compared with the classical approaches,[9,10] the construction of univariate polynomial equation for lattice constant c in the pGHQ scheme is systematical and general, supporting

symmetric and asymmetric lattices and covering all quadrature degrees. The procedure is concise without involving co-solving of c and $\{w_\alpha\}$. It can be mathematically proven that the univariate polynomial equation of c in Refs. [9] and [10] equals HCES. Here, a justification for the Shan scheme[9] is offered in Section 3 of the Supplementary Material. It is also worth noting that though pGHQ is proposed for the Hermite polynomial expansion theory, it can also be extended into entropic LB model. Actually, it is the mathematical mechanism of a popular entropic LB discretization, the Karlin–Asinari scheme.[11] The detailed justification can be found in Section 4 of the Supplementary Material. This explains the interesting question[9]—why, for a given discrete velocity set, does one get the same lattice constant and weights under different schemes, even under different theories?

3. Application

Since the pGHQ scheme offers a series of HCES covering the full-range quadrature degree and supports all kinds of lattices, a direct application is to construct optimal lattices, which restores the same moment degree with the smallest discrete velocity set. In terms of the pGHQ scheme, given an nth-order moment degree on-node ED discretization, it is to construct a discrete velocity set $\{v_0,\ldots,v_{q-1}\}$ with the smallest q, whose $q\sim(2n-q)^{\text{th}}$ HCES has real-valued solution for lattice constant c. The theoretically smallest number for q is $(n+1)$, which indicates that its corresponding abscissa polynomial can be expressed as

$$W_{(n+1)}(\xi)=\frac{1}{2^{n+1}}H_{n+1}(\xi)+A_nH_n(\xi). \tag{16}$$

Unfortunately, the mechanism of tuning the coefficient A_n to generate desirable zeros, which can fit into nodes, is not clear. Hence, the global optimal lattices are not available right now. However, since the procedure of the pGHQ scheme is unified for both symmetric and asymmetric, and the core computation is solving HCES which is a univariate polynomial equation system, the pGHQ scheme is extremely suitable for computers. Therefore, limiting the range of the discrete velocity, a brute-force approach is available, which is to enumerate all of the possible discrete velocity sets and identify their feasibilities. Here, we search the local optimal lattices on $[-10,10]$ for $\{n=3,4,5,6,7\}$ moment degree ED discretization. The detailed procedures of searching local optimal lattices on $[-m,m]$ for u^n ED discretization are:

(I) set up q, start up with the theoretically smallest number $q=n+1$;

(II) enumerate all the possible q-point discrete velocity sets on $[-m,m]$;

(III) solve $q\sim(2n-q)^{\text{th}}$ HCES for each enumerated discrete velocity set. Identify the set with real-valued c as feasible lattices;

(IV) all the identified feasible sets are local optimal lattices on $[-m,m]$. If there is no feasible lattice in the enumerated sets, then increase q by 1, repeat steps (II)–(IV).

We find that all of these local optimal lattices keep the symmetric form, $\{0,\pm v_1,...,\pm v_{n-1}\}$. The local optimal abscissa number q on $[-10,10]$ has the relationship $q=2n-1$ with the moment degree n. To verify the feasibility of asymmetric lattices, we continue our search with an extra point. The search shows that for a given n moment degree ED discretization, the available lattices are extremely abundant. Taking $n=3$ moment degree ED discretization as an instance, in the range $[-10,10]$, there are 20 5-point lattices (local optimal lattices) whose discrete velocity set has the form $\{0,\pm v_1,\pm v_2\}$ and 34636 6-point lattices, where most of them are asymmetric lattices. Table 1 lists the detailed statistics of our search. As a detailed illustration of the local optimal lattices, Table 2 presents the most compact local optimal lattices on $[-10,10]$ for $\{n=3,4,5,6,7\}$ moment degree ED discretization, whose discrete velocity is as close as possible to 0. To give a specific display of the abundance of the available lattices, Tables 3 and 4 list several symmetric and asymmetric lattices of $n=3$ moment degree ED discretization.

Table 1. Statistics of the available on-node lattices for $\{n=3,4,5,6,7\}$ moment degree ED discretization on the interval $[-10,10]$. The local optimal q, the total number of available local optimal lattices, and the total number of available $(q+1)$-point lattices are respectively listed in columns 2, 3, and 4 of the table.

Moment degree u^n	Local optimal q	q-point lattices	$(q+1)$-point lattices
3	5	20	34636
4	7	120	138715
5	9	112	244218
6	11	252	211863
7	13	112	82684

Table 2. The most compact local optimal on-node lattices on $[-10,10]$ for $\{n=3,4,5,6,7\}$ moment degree ED discretization.

Moment degree u^n	Lattices $\{v_0,\pm v_1,\cdots\}$	Lattice constant c	weights $\{w_0,w_1,\cdots\}$
3	$\{0,\pm1,\pm3\}$	1.1664	$\{6.3665\times10^{-1},1.8141\times10^{-1},2.6196\times10^{-4}\}$
		5.5343×10^{-1}	$\{7.4464\times10^{-2},4.1859\times10^{-1},4.4182\times10^{-2}\}$
4	$\{0,\pm1,\pm2,\pm3\}$	8.4639×10^{-1}	$\{4.7667\times10^{-1},2.3391\times10^{-1},2.6938\times10^{-2},8.1213\times10^{-4}\}$
5	$\{0,\pm1,\pm2,\pm3,\pm5\}$	8.1321×10^{-1}	$\{4.5814\times10^{-1},2.3734\times10^{-1},3.2325\times10^{-2},1.2641\times10^{-3},8.9773\times10^{-7}\}$
		4.7942×10^{-1}	$\{1.6724\times10^{-1},3.0315\times10^{-1},5.3303\times10^{-2},5.7922\times10^{-2},2.0013\times10^{-3}\}$
6	$\{0,\pm1,\pm2,\pm3,\pm4,\pm5\}$	6.8590×10^{-1}	$\{3.8694\times10^{-1},2.4178\times10^{-1},5.8922\times10^{-2},5.6153\times10^{-3},2.0652\times10^{-4},3.2745\times10^{-6}\}$
7	$\{0,\pm1,\pm2,\pm3,\pm4,\pm5,\pm7\}$	6.6344×10^{-1}	$\{3.7428\times10^{-1},2.4105\times10^{-1},6.4343\times10^{-2},7.1316\times10^{-3},3.2523\times10^{-4},6.6163\times10^{-6},3.0509\times10^{-9}\}$
		4.3240×10^{-1}	$\{2.0928\times10^{-1},2.3312\times10^{-1},9.4051\times10^{-2},5.6923\times10^{-2},7.5008\times10^{-3},3.7006\times10^{-3},6.0784\times10^{-5}\}$

Table 3. All the available local optimal on-node lattices for $n=3$ moment degree ED discretization on the interval $[-5,5]$. All feasible discrete velocity sets keep the symmetric form, $\{0,\pm v_1,\pm v_2\}$. The v_α and $-v_\alpha$ share the same weight w_α. Each feasible lattice has two lattice constants. To save space, the two lattice constants c and their corresponding weights $\{w_0,w_1,w_2\}$ are denoted by the symbols $\mp$ and $\pm$. The rational form is kept for comparison with the existing ED discretizations.

$\{0,\pm v_1,\pm v_2\}$	c	w_0	w_1	w_2
$\{0,\pm1,\pm3\}$	$\sqrt{(5\mp\sqrt{10})}/\sqrt{6}$	$4\left(4\mp\sqrt{10}\right)/45$	$3\left(8\pm\sqrt{10}\right)/80$	$\left(16\pm5\sqrt{10}\right)/720$
$\{0,\pm1,\pm4\}$	$\sqrt{51\mp\sqrt{1641}}/8$	$\left(93\mp17\sqrt{1641}\right)/1200$	$\left(1959\pm29\sqrt{1641}\right)/4500$	$\left(933\pm23\sqrt{1641}\right)/36000$
$\{0,\pm1,\pm5\}$	$\sqrt{39\mp\sqrt{1146}}/5\sqrt{2}$	$\left(-528\mp52\sqrt{1146}\right)/1875$	$\left(2208\pm47\sqrt{1146}\right)/3600$	$\left(2472\pm73\sqrt{1146}\right)/90000$
$\{0,\pm2,\pm5\}$	$\sqrt{87\mp\sqrt{1569}}/20$	$\left(3477\mp29\sqrt{1569}\right)/7500$	$\left(3153\pm19\sqrt{1569}\right)/12600$	$\left(2829\pm67\sqrt{1569}\right)/157500$

Table 4. The available asymmetric on-node lattices for $n=3$ moment degree ED discretization.

$\{v_0,v_1,...,v_5\}$	c	w_0	w_1	w_2	w_3	w_4	w_5
$\{-5,-2,-1,1,2,4\}$	0.381641	0.019568	0.302751	0.094520	0.505439	0.009237	0.068487
$\{-4,-3,-1,1,2,4\}$	0.450877	0.016717	0.054744	0.451349	0.323613	0.127736	0.025841
$\{-3,-1,0,1,2,4\}$	0.521696	0.059199	0.366034	0.198867	0.227904	0.138130	0.009866
$\{-3,-1,0,1,2,5\}$	0.553432	0.076212	0.294489	0.352957	0.040448	0.232265	0.003629

4. Implication

A direct implication of lattices abundance is its impact on the positivity of equilibrium distribution; i.e., the range of macro velocity on which all equilibrium distributions remains positive. Because a negative equilibrium distribution violates the physical nature of particle kinetics, the positivity is considered as a major factor for the numerical stability of the LB method. We have analyzed lattices $\{0,\pm1\}$, $\{0,\pm2,\pm5\}$, $\{0,\pm1,\pm3\}$, $\{0,\pm1,\pm2,\pm3\}$, $\{0,\pm1,\pm2,\pm3,\pm5\}$, and $\{0,\pm1,\pm2,\pm3,\pm4,\pm5\}$. For lattices $\{0,\pm2,\pm5\}$, $\{0,\pm1,\pm3\}$, $\{0,\pm1,\pm2,\pm3,\pm5\}$ have two feasible lattice constants c, we take the c with a wider positivity. The analysis shows that lattice $\{0,\pm2,\pm5\}$ has the widest positivity though its retained moment degree is only u^3.

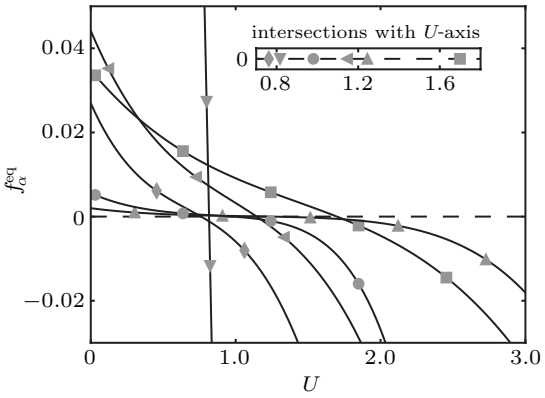


Fig. 1. The profiles of first-going-negative equilibrium distributions f_α^{eq} as a function of U. The figure only renders the positive U-axis. Since all lattices in the figure are symmetric, the positivity on the negative U-axis is the same though the corresponding v_α turns to $-v_\alpha$. The line with symbol ▼ is for f_α^{eq} with $v_\alpha=0$ and $c=1/\sqrt{2RT}=1.2247$ which, as U increases, first goes negative in all equilibrium distributions of $\{0,\pm1\}$; ■ is for $v_\alpha=-5$ and $c=0.3442$ in $\{0,\pm2,\pm5\}$; ◀ is for $v_\alpha=-3$ and $c=0.5534$ in $\{0,\pm1,\pm3\}$; ♦ is for $v_\alpha=-2$ and $c=0.8464$ in $\{0,\pm1,\pm2,\pm3\}$; ▲ is for $v_\alpha=-5$ and $c=0.4794$ in $\{0,\pm1,\pm2,\pm3,\pm5\}$; • is for $v_\alpha=-3$ and $c=0.6859$ in $\{0,\pm1,\pm2,\pm3,\pm4,\pm5\}$. The inner panel renders their intersections with the U-axis, above which the f_α^{eq} will become negative. The specific values of intersections for $\{▼,■,◀,♦,▲,•\}$ are $\sim\{0.82, 1.70, 1.15, 0.76, 1.25, 0.98\}$. Since the plotted f_α^{eq} curves are the first-going-negative equilibrium distributions, then the inner panel demonstrates the lattices positivity range of U.

Meanwhile, the positivity of the highest retaining-moment-degree lattice $\{0,\pm1,\pm2,\pm3,\pm4,\pm5\}$ is merely better than $\{0,\pm1\}$ and $\{0,\pm1,\pm2,\pm3\}$. To demonstrate it, figure 1 plots their equilibrium distributions which firstly go negative as the macro velocity increases. The asymmetric lattice also demonstrates its capability on modifying the positivity on a specific range of U. Figure 2 plots a comparison of lattices $\{-5,-2,-1,1,2,4\}$ and $\{0,\pm2,\pm5\}$. This shows that the lattice $\{-5,-2,-1,1,2,4\}$ shifts the positivity range of $\{0,\pm2,\pm5\}$ left with approximatively -0.5 on the U-axis. This analysis indicates that the discrete velocity set could be a significant impact to the numerical stability of LB method. It offers a direction to improve LB numerical stability. Our identified lattices also offer a database for further study. However, a detailed investigation is beyond the scope of this paper and shall be addressed in a separate publication.

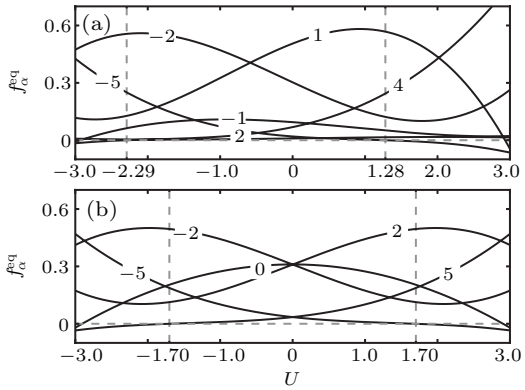


Fig. 2. The profiles of equilibrium distributions f_α^{eq} as a function of U: (a) lattice $\{-5,-2,-1,1,2,4\}$ with a lattice constant $c=0.3816$; (b) lattice $\{0,\pm2,\pm5\}$ with a lattice constant $c=0.3442$. The label on a curve is its corresponding v_α. The intervals of U between vertical dashed lines are lattices positivity ranges.

5. Conclusion

We propose a new mathematical tool, pGHQ, to construct on-node LB lattices under a Cartesian coordinate system in this paper. To the best of our knowledge, this is the first time

to derive and employ this mathematical tool in the context of the LB method. The pGHQ is general. It can be extended into the entropic LB model, even though it was first proposed for the Hermite polynomial expansion theory. The pGHQ scheme avoids the tedious QES solving. Compared with the existing classical approaches, our scheme has the following advantages: (i) the algorithm is extremely concise; (ii) the procedure of constructing univariate polynomial equations is unified for both symmetric and asymmetric lattices; and (iii) the generated univariate polynomial equation system covers full-range quadrature degree of the given $\{v_0,\ldots,v_{q-1}\}$. We employ the pGHQ scheme to search the local optimal and asymmetric lattices on $[-10,10]$ for $\{n=3,4,5,6,7\}$ moment degree ED discretization. The search reveals a surprising abundance of available lattices. Our brief analysis shows that the discrete velocity set is significant to the positivity of equilibrium distribution, which is one major impact to the numerical stability of LB method. Hence, the results of the pGHQ scheme lay a foundation for further investigation to improve the numerical stability of the LB method by modifying the discrete velocity set.

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