Bias in the direct numerical simulation of isotropic turbulence using the lattice Boltzmann method

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(Received 24 May 2004; revised manuscript received 11 October 2004; published 17 March 2005)

Direct numerical simulation of homogeneous, isotropic turbulence using the lattice Boltzmann method is revised. Two-point pressure and velocity correlations are studied and analytical results are derived taking into account the dynamics of the lattice Boltzmann equation. Using the parameters of a two-dimensional (D2Q9) and a three-dimensional (D3Q19) model, it is demonstrated that correlation functions obtained from lattice Boltzmann simulations may have systematic errors at large separation distances due to the second-order error terms.

DOI: 10.1103/PhysRevE.71.036705 PACS number(s): 02.70.−c, 47.35.+i, 47.40.−x

I. INTRODUCTION

Direct numerical simulation is a standard tool in turbulence research [1]. It is generally admitted that, using direct numerical simulation, one has to resolve all the energy-containing scales of the flow, i.e., the smallest one has to be on the order of η, which is the Kolmogorov scale [2]. Since in such simulations the numerical methods are required to reproduce all the scales accurately, spectral methods were used almost exclusively in the beginning of the numerical turbulence research. However, due to the development of fast, low-storage new numerical algorithms, the privilege of spectral methods seems to be over, and nowadays it is not difficult to find direct numerical simulations, where finite difference or discrete kinetic schemes are in action. For instance, Benzi *et al.* [3] used the lattice Boltzmann method to study the scaling properties of the structure functions in anisotropic homogeneous turbulence. Fogaccia *et al.* [4] extended the lattice Boltzmann method to study plasma turbulence. Amati *et al.* [5] simulated fully developed turbulence and recently Cosgrove *et al.* [6] studied flow instabilities in a channel using the lattice Boltzmann approach.

In this paper we study the fundamental equation of the method used by Benzi *et al.* [3], *viz.*, the lattice Boltzmann equation with the BGK (Bhatnagar-Gross-Krook) collision operator. This collision operator describes a single relaxation process to an interpolated Maxwell-Boltzmann equilibrium. The correlations between the equilibrium distributions play a major role in the analysis. So, first the two-point correlation functions between the equilibrium distributions will be derived considering homogeneous and isotropic turbulence. Then, it will be shown how these correlations give rise to two-point correlations between the macroscopic quantities such as the pressure and the velocity. It will be pointed out that the well-known form of the two-point pressure and velocity correlations can be obtained in the low Mach number limit, and these correlations do not contain systematic deviations up to the accuracy of the method considered. However, in the second-order error some terms scale with the separation distance, and these terms may cause systematic deviations in the correlation functions.

II. THE LATTICE BOLTZMANN METHOD

For completeness, let us briefly recall some basic facts on the lattice Boltzmann method (for details see Ref. [7]).

Using the lattice Boltzmann method (LBM), one solves a discrete kinetic equation for the one-particle velocity distribution functions f_i-*s* [8,9]

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta x, t+\Delta t) - f_i(\mathbf{x},t) = \Omega_i, \tag{1}$$

where $\mathbf{c}_i$ is the lattice vector, Δx is the lattice spacing, Δt is the time step, and Ω_i is the collision operator.

In this paper we use the simplest form of the latter, i.e., the BGK operator [10,11]

$$\Omega_i = -\frac{1}{\tau}[f_i(\mathbf{x},t) - f_i^{eq}(\mathbf{x},t)],$$

where τ is the relaxation time and f_i^{eq} is an equilibrium distribution function. The equilibrium distribution function can take the following form [12]:

$$f_i^{eq} = w_i\left[p + p_0\left[\frac{c_{i\alpha}u_\alpha}{c_s^2} + \frac{u_\alpha u_\beta}{c_s^4}(c_{i\alpha}c_{i\beta} - c_s^2\delta_{\alpha\beta})\right]\right], \tag{2}$$

where w_i is the lattice weight, $p=\rho c_s^2$ is the pressure, $p_0=\rho_0 c_s^2$ is the reference pressure, u is the hydrodynamic velocity, and c_s is the speed of sound (repeated Greek indices imply summation).

Solving Eq. (1), one can obtain the macroscopic quantities by taking the suitable moments of the distribution functions

$$p = \sum_i f_i, \quad p_0 u_\alpha = \sum_i c_{i\alpha} f_i.$$

For a specific model, the lattice vector and the lattice weights need to be selected. In our analysis we will use the parameters of a two-dimensional, nine-velocity model (D2Q9) and a three-dimensional, 19-velocity model (D3Q19) [13].

For these models, the lattice links and the corresponding weights are defined as follows:

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$$\mathbf{c}_0^{D2Q9} = (0,0) \quad w_0^{D2Q9} = \frac{4}{9}$$

$$\mathbf{c}_{1,\ldots,6}^{D2Q9} = (\pm 1,0),(0,\pm 1) \quad w_{1,\ldots,6}^{D2Q9} = \frac{1}{9}$$

$$\mathbf{c}_{7,\ldots,18}^{D2Q9} = (\pm 1,\pm 1) \quad w_{7,\ldots,18}^{D2Q9} = \frac{1}{36}$$

and

$$\mathbf{c}_0^{D2Q19} = (0,0,0)$$

$$\mathbf{c}_{1,\ldots,6}^{D2Q19} = (\pm 1,0,0),(0,\pm 1,0),(0,0,\pm 1)$$

$$\mathbf{c}_{7,\ldots,18}^{D2Q19} = (\pm 1,\pm 1,0),(\pm 1,0,\pm 1),(0,\pm 1,\pm 1)$$

$$w_0^{D2Q19} = \frac{1}{3}$$

$$w_{1,\ldots,6}^{D2Q19} = \frac{1}{18}$$

$$w_{7,\ldots,18}^{D2Q19} = \frac{1}{36}.$$

Using Chapman-Enskog expansion, one can show that the solution of Eq. (1) results in solutions of the incompressible Navier-Stokes equations with some errors. The errors are in relation to the finite lattice spacing, time step, and Mach number. Basically, the lattice Boltzmann method is a second-order numerical method for the Navier-Stokes equation in the low Mach number limit. The method can be simplified significantly if the relaxation time $\tau=1$. Then, the LBE takes the form

$$f_i(\mathbf{x},t) = f_i^{eq}(\mathbf{x} - \mathbf{c}_i\Delta x, t - \Delta t). \tag{3}$$

Note that this form establishes relations between macroscopic quantities implicitly. First, for simplicity, we will use this form of the lattice Boltzmann equation, but later our analysis will be extended considering the influence of the nonequilibrium distributions.

It is worth mentioning that in lattice Boltzmann models the relaxation time is in direct relation with the viscosity and, in practice, the simplification above would prescribe strict lower and upper limits for the available viscosity and Reynolds number, respectively. However, in our analysis the domain size is not limited and consequently we can consider arbitrarily high Reynolds numbers.

III. CORRELATIONS BETWEEN EQUILIBRIUM DISTRIBUTIONS

The correlations between the equilibrium distributions separated by a vector $\mathbf{r}$ can be written as follows:

$$B_{ij}^{eq}(\mathbf{r}) = \langle f_i^{eq}(\mathbf{x}) f_j^{eq}(\mathbf{x}+\mathbf{r})\rangle, \tag{4}$$

where the operator $\langle \ldots \rangle$ means ensemble averaging.

Without the loss of generality, we can assume that the reference pressure $p_0=1$. Substitution of the equilibrium distribution functions into Eq. (4) yields

$$\begin{aligned} B_{ij}^{eq}(r) = \Gamma_{ij}\langle &[p(\mathbf{x}) + \Psi_{i\alpha}u_\alpha(\mathbf{x}) + \Phi_{i\alpha\beta}u_\alpha(\mathbf{x})u_\beta(\mathbf{x})] \\ &\times[p(\mathbf{x}+\mathbf{r}) + \Psi_{j\gamma}u_\gamma(\mathbf{x}+\mathbf{r}) \\ &+ \Phi_{j\gamma\eta}u_\gamma(\mathbf{x}+\mathbf{r})u_\eta(\mathbf{x}+\mathbf{r})]\rangle, \end{aligned} \tag{5}$$

where we introduced the following quantities:

$$\Gamma_{ij} = w_i w_j, \quad \Psi_{i\alpha} = \frac{c_{i\alpha}}{c_s^2}, \quad \Phi_{i\alpha\beta} = \frac{c_{i\alpha}c_{i\beta} - c_s^2\delta_{\alpha\beta}}{c_s^4}.$$

A. Homogeneous turbulence

Assuming homogeneity, the right-hand side of Eq. (5) can be rewritten as follows:

$$\begin{aligned} B_{ij}^{eq}(\mathbf{r}) = \Gamma_{ij}[&T_{ij0}(\mathbf{r}) + T_{ij1}(\mathbf{r}) + T_{ij2}(\mathbf{r}) + T_{ij3}(\mathbf{r}) + T_{ij4}(\mathbf{r}) \\ &+ T_{ij5}(\mathbf{r})], \end{aligned} \tag{6}$$

where

$$T_{ij0}(\mathbf{r}) = B_{p,p}(\mathbf{r}),$$

$$T_{ij1}(\mathbf{r}) = \Psi_{i\alpha}B_{\alpha,p}(\mathbf{r}) + \Psi_{j\alpha}B_{p,\alpha}(\mathbf{r}),$$

$$T_{ij2}(\mathbf{r}) = \Phi_{i\alpha\beta}B_{\alpha\beta,p}(\mathbf{r}) + \Phi_{j\alpha\beta}B_{p,\alpha\beta}(\mathbf{r}),$$

$$T_{ij3}(\mathbf{r}) = \Psi_{i\alpha}\Psi_{j\beta}B_{\alpha,\beta}(\mathbf{r}),$$

$$T_{ij4}(\mathbf{r}) = \Phi_{i\alpha\beta}\Psi_{j\gamma}B_{\alpha\beta,\gamma}(\mathbf{r}) + \Phi_{j\alpha\beta}\Psi_{i\gamma}B_{\gamma,\alpha\beta}(\mathbf{r}),$$

$$T_{ij5}(\mathbf{r}) = \Phi_{i\alpha\beta}\Phi_{j\gamma\eta}B_{\alpha\beta,\gamma\eta}(\mathbf{r}).$$

Here, Bs are two-point correlations between the corresponding macroscopic quantities, i.e.,

$$B_{p,p}(\mathbf{r}) = \langle p(\mathbf{x})p(\mathbf{x}+\mathbf{r})\rangle,$$

$$B_{p,\alpha} = \langle p(\mathbf{x})u_\alpha(\mathbf{x}+\mathbf{r})\rangle,$$

$$B_{\alpha,p} = \langle u_\alpha(\mathbf{x})p(\mathbf{x}+\mathbf{r})\rangle,$$

$$B_{\alpha\beta,p}(\mathbf{r}) = \langle u_\alpha(\mathbf{x})u_\beta(\mathbf{x})p(\mathbf{x}+\mathbf{r})\rangle,$$

$$B_{p,\alpha\beta}(\mathbf{r}) = \langle p(\mathbf{x})u_\alpha(\mathbf{x}+\mathbf{r})u_\beta(\mathbf{x}+\mathbf{r})\rangle,$$

$$B_{\alpha,\beta}(\mathbf{r}) = \langle u_\alpha(\mathbf{x})u_\beta(\mathbf{x}+\mathbf{r})\rangle,$$

$$B_{\alpha\beta,\gamma}(\mathbf{r}) = \langle u_\alpha(\mathbf{x})u_\beta(\mathbf{x})u_\gamma(\mathbf{x}+\mathbf{r})\rangle,$$

$$B_{\gamma,\alpha\beta}(\mathbf{r}) = \langle u_\gamma(\mathbf{x})u_\alpha(\mathbf{x}+\mathbf{r})u_\beta(\mathbf{x}+\mathbf{r})\rangle,$$

$$B_{\alpha\beta,\gamma\eta}(\mathbf{r}) = \langle u_\alpha(\mathbf{x})u_\beta(\mathbf{x})u_\gamma(\mathbf{x}+\mathbf{r})u_\eta(\mathbf{x}+\mathbf{r})\rangle.$$

B. Isotropic turbulence

In the case of homogeneous, isotropic turbulence, the two-point correlations can depend only on the distance be-

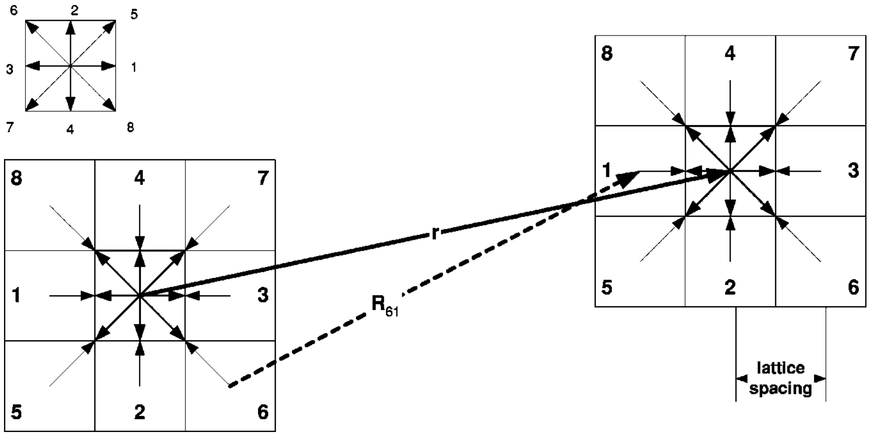

FIG. 1. Indices of the lattice links are shown for a D2Q9 model (left top). The base separation vector and the nearest neighbors are shown with the separation vector of the sixth and first link correlations.

tween the points considered, and the terms in the correlation functions of the equilibrium distributions can be rewritten using the well-known forms of two-point correlation tensors for homogeneous, isotropic fields [14]

$$T_{ij0}(\mathbf{r}) = Q(r),$$

$$T_{ij1}(\mathbf{r}) = \Pi^1_{ij,\alpha}\frac{r_\alpha}{r}D(r),$$

$$T_{ij2}(\mathbf{r}) = \Pi^2_{ij,\alpha\beta}[E_1(r)r_\alpha r_\beta + E_2(r)\delta_{\alpha\beta}],$$

$$T_{ij3}(\mathbf{r}) = \Pi^3_{ij,\alpha\beta}[A_1(r)r_\alpha r_\beta + A_2(r)\delta_{\alpha\beta}],$$

$$T_{ij4}(\mathbf{r}) = \Pi^4_{ij,\alpha\beta\gamma}[B_1(r)r_\alpha r_\beta r_\gamma + B_2(r)(\delta_{\beta\gamma}r_\alpha + \delta_{\alpha\gamma}r_\beta) + B_3(r)\delta_{\alpha\beta}r_\gamma],$$

$$T_{ij5}(\mathbf{r}) = \Pi^5_{ij,\alpha\beta\gamma\eta}[C_1(r)r_\alpha r_\beta r_\gamma r_\eta + C_2(r)(r_\alpha r_\beta\delta_{\gamma\eta} + r_\gamma r_\eta\delta_{\alpha\beta}) + C_3(r)(r_\alpha r_\gamma\delta_{\beta\eta} + r_\alpha r_\eta\delta_{\beta\gamma} + r_\beta r_\gamma\delta_{\alpha\eta} + r_\beta r_\eta\delta_{\alpha\gamma}) + C_4(r)(\delta_{\alpha\gamma}\delta_{\beta\eta} + \delta_{\alpha\eta}\delta_{\beta\gamma}) + C_5(r)\delta_{\alpha\beta}\delta_{\gamma\eta}], \quad (7)$$

where $Q(r)$, $A_{1,\ldots,2}(r)$, $B_{1,\ldots,3}(r)$, $C_{1,\ldots,5}(r)$, $D(r)$, and $E_{1,\ldots,2}(r)$ are some unknown scalar functions and

$$\Pi^{(1)}_{ij,\alpha} = \Psi_{i\alpha} - \Psi_{j\alpha}, \quad \Pi^{(2)}_{ij,\alpha\beta} = \Phi_{j\alpha\beta} + \Phi_{i\alpha\beta},$$

$$\Pi^{(3)}_{ij,\alpha\beta} = \Psi_{i\alpha}\Psi_{j\beta}, \quad \Pi^{(4)}_{ij,\alpha\beta\gamma} = \Phi_{i\alpha\beta}\Psi_{j\gamma} - \Phi_{j\alpha\beta}\Psi_{i\gamma},$$

$$\Pi^{(5)}_{ij,\alpha\beta\gamma\eta} = \Phi_{i\alpha\beta}\Phi_{j\gamma\eta}. \quad (8)$$

To obtain (7) and (8) homogeneity of the fields was used, implying, for instance, that $B_{p,\alpha}(\mathbf{r}) = B_{\alpha,p}(-\mathbf{r})$ and, since $B_{\alpha,p}(\mathbf{r}) = (r_\alpha/r)D(r)$, therefore $B_{p,\alpha}(\mathbf{r}) = -(r_\alpha/r)D(r)$ [14].

IV. MACROSCOPIC CORRELATIONS IN HOMOGENEOUS, ISOTROPIC TURBULENCE

Let us consider a lattice Boltzmann simulation of a homogeneous, isotropic turbulent flow where the lattice spacing is fine enough to resolve all the relevant scales of the turbulent field. Considering the simplest form of the lattice Boltzmann equation, i.e., Eq. (3), the macroscopic quantities are given by the moments of the distribution functions at time t

$$p(\mathbf{x},t) = \sum_i f_i^{eq}(\mathbf{x} - \mathbf{c}_i\Delta x, t - \Delta t),$$

$$u_\alpha(\mathbf{x},t) = \sum_i c_{i\alpha} f_i^{eq}(\mathbf{x} - \mathbf{c}_i\Delta x, t - \Delta t).$$

It is worth noting that in the previous sections we worked with continuous **x** and **r**, but here we consider both **x** and **r** on a lattice space.

A. Two-point pressure correlation

Thus, the two-point pressure correlation can be written as follows:

$$\tilde{B}_{p,p}(\mathbf{r},t) = \langle p(\mathbf{x},t)p(\mathbf{x}+\mathbf{r},t)\rangle = \left\langle \left[\sum_i f_i^{eq}(\mathbf{x} - \mathbf{c}_i\Delta x, t - \Delta t)\right] \times \left[\sum_j f_j^{eq}(\mathbf{x} + \mathbf{r} - \mathbf{c}_j\Delta x, t - \Delta t]\right\rangle.$$

Assuming statistical stationarity, we can drop the time arguments, obtaining

$$\tilde{B}_{p,p}(\mathbf{r}) = \sum_i \sum_j \langle f_i^{eq}(\mathbf{x} - \mathbf{c}_i\Delta x) f_j^{eq}(\mathbf{x} + \mathbf{r} - \mathbf{c}_j\Delta x)\rangle = \sum_{i,j} B_{ij}^{eq}(\mathbf{R}_{ij}).$$

As one can see, the pressure correlation can be expressed by the combination of equilibrium distribution correlations, where $\mathbf{R}_{ij} = \mathbf{r} + \Delta x(\mathbf{c}_i - \mathbf{c}_j)$ (see Fig. 1).

Using Eq. (6), one obtains

$$\tilde{B}_{p,p}(\mathbf{r}) = \sum_{i,j,k} \Gamma_{ij} T_{ijk}(\mathbf{R}_{ij}), \quad (9)$$

where, e.g.,

$$T_{ij1}(\mathbf{R}_{ij}) = \Pi^{(1)}_{ij,\alpha}\frac{R_{ij,\alpha}}{R_{ij}}D(R_{ij}),$$

and $R_{ij} = |\mathbf{R}_{ij}|$ is the length of the separation vector.

Expressing the lattice Boltzmann pressure correlation $\widetilde{B}_{p,p}(\mathbf{r})$ by the terms of Eq. (9), one has to get back the base correlation $B_{p,p}(\mathbf{r})=Q(r)$, which depends only on r. Due to the finite lattice spacing the result is somewhat more complicated, since terms involving Δx in the function arguments also appear in the correlation.

Taking the Taylor expansion of the correlation function $\widetilde{B}_{p,p}(r)$ and keeping only the leading and first-order terms, one can obtain

$$\widetilde{B}_{p,p} = Q + 2\frac{\lambda D + rD'}{r}\Delta x + O(\Delta x^2), \tag{10}$$

where the prime is for derivatives with respect to r, i.e., $D' = dD/dr$, $\lambda=1$, and $\lambda=2$ for the D2Q9 and the D3Q19 models, respectively.

So, we have found that the two-point pressure correlation is given by Eq. (10) in the lattice Boltzmann models considered here. During the derivation we presumed that the correlations have their perfect isotropic forms in the neighborhood of the two points in question. This is an ideal situation.

Using this assumption, we obtained a first-order error term in the two-point pressure correlation, and the error term is in relation to the scalar function of the two-point mixed pressure-velocity correlation, i.e., $D(r)$. A brief analysis can show that the term disappears in the low Mach number limit. Indeed, the term is zero if the function $D(r)$ satisfies the following differential equation:

$$\lambda D/r + D' = 0. \tag{11}$$

Since the solution of this equation is given by $D(r)=cr^{-\lambda}$, which becomes infinite at $r=0$ and $c \neq 0$, therefore $D(r)=0$ is the only possible solution. Actually, this is a well-known result of classical analysis of isotropic fields; the mixed correlation vanishes in incompressible flows [14]. Since the lattice Boltzmann models studied here work in the low Mach number limit, this result is in line with the standard theory.

B. Two-point velocity correlation

In the same way, we can derive the two-point velocity correlation function.

The two-point velocity correlation can be given as follows:

$$\begin{aligned}\langle u_\alpha(\mathbf{x})u_\beta(\mathbf{x}+\mathbf{r})\rangle &= \left\langle \left[\sum_i c_{i\alpha} f_i^{eq}(\mathbf{x}-\mathbf{c}_i\Delta x)\right] \times \left[\sum_j c_{j\beta} f_j^{eq}(\mathbf{x}+\mathbf{r}-\mathbf{c}_j\Delta x)\right]\right\rangle \\ &= \sum_{i,j} c_{i\alpha}c_{j\beta}B_{ij}^{eq}(\mathbf{R}_{ij}).\end{aligned}$$

Using Eq. (6), one obtains

$$\widetilde{B}_{\alpha,\beta}(\mathbf{r}) = \sum_{i,j,k} c_{i\alpha}c_{j\beta}\Gamma_{ij}T_{ij,k}(\mathbf{R}_{ij}).$$

Now, one can take the Taylor expansion of the above correlation and, keeping only the leading and first-order terms, the correlation can be written as follows:

$$\widetilde{B}_{\alpha,\beta} = (A_1 r_\alpha r_\beta + A_2\delta_{\alpha\beta}) + \{4\delta_{\alpha\beta}(\kappa B_2 + rB_2' + B_3) + 4r_\alpha r_\beta \times[(\kappa+1)B_1 + rB_1' + r^{-1}(B_2'+B_3')]\}\Delta x + O(\Delta x^2), \tag{12}$$

where $\kappa=3$ and $\kappa=4$ for the D2Q9 and the D3Q19 model, respectively.

It is worth noting that to obtain Eq. (12) we assumed that the scalar function of the mixed correlation $D(r)$ vanishes. This assumption is justified for incompressible flows, as we demonstrated in the previous section.

The longitudinal correlation function can be obtained by rewriting Eq. (12)

$$\widetilde{B}_{L,L} = (A_1 r^2 + A_2) + \{4(\kappa B_2 + rB_2' + B_3) + 4r^2[(\kappa+1)B_1 + rB_1' + r^{-1}(B_2'+B_3')]\}\Delta x + O(\Delta x^2). \tag{13}$$

For a solenoidal velocity field, the scalar functions of the third moments satisfy the following relations [14]:

$$B_1 = \frac{1}{r}B_3', \quad B_2 = -\frac{3}{2}B_3 - \frac{r}{2}B_3'. \tag{14}$$

Substitution of the relations (14) into Eq. (13) yields

$$\widetilde{B}_{L,L} = B_{L,L} + 4\left[B_3\left(1-\frac{3}{2}\kappa\right) + B_3' r\left(\frac{1}{2}\kappa - 3\right)\right]\Delta x + O(\Delta x^2). \tag{15}$$

In order to express the deviation of the two-point velocity correlation of the lattice Boltzmann simulation in terms of $B_{L,L}$, we can use the von Kármán–Howarth equation, which forms a relation between the second and third moment [14]

$$\frac{\partial B_{L,L}(r,t)}{\partial t} = \left(\frac{\partial}{\partial r} + \frac{4}{r}\right)\left[B_{LL,L}(r,t) + 2\upsilon\frac{\partial B_{L,L}(r,t)}{\partial r}\right], \tag{16}$$

where the longitudinal third-order correlation can be written as follows [14]:

$$B_{LL,L} = B_1 r^3 + (2B_2 + B_3)r. \tag{17}$$

Using the relations (14), one can obtain

$$B_{LL,L} = -2rB_3. \tag{18}$$

Considering statistical steady state and substituting the third-order correlation into Eq. (16), the following ordinary differential equation can be derived:

$$\left(\frac{d}{dr} + \frac{4}{r}\right)(rB_3) = \nu\left(\frac{d}{dr} + \frac{4}{r}\right)\frac{dB_{L,L}}{dr.} \tag{19}$$

The solution of the above ordinary differential equation is given by

$$B_3(r) = \frac{r^{-5}}{6}\left[\int \Delta x r^3(rB''_{L,L} + 4B'_{L,L})dr + c\right], \quad (20)$$

where we used that the kinematic viscosity is given by $\nu = \Delta x/6$ in the case of $\tau = 1$ for the models in question, and c is a constant.

Substitution of Eq. (20) into Eq. (15) yields

$$B_3\left(1 - \frac{3}{2}\kappa\right) + B'_3 r\left(\frac{1}{2}\kappa - 3\right) = \frac{1}{12}[(\kappa - 6)\Delta x(B''_{L,L} + 4B'_{L,L}r^{-1}) + 8r^{-5}(4 - \kappa)(6c + \Delta x I)],$$

where

$$I = \int r^3(rB''_{L,L} + 4B'_{L,L})dr.$$

Using integration by parts, one can see that

$$\int r^4 B''_{L,L}dr = r^4 B'_{L,L} - 4\int r^3 B'_{L,L}dr,$$

therefore

$$I = r^4 B'_{L,L}.$$

The LBM correlation can be rewritten as follows:

$$\tilde{B}_{L,L} = B_{L,L} + \phi_1 r^{-5}\Delta x + \phi_2 r^{-1}\Delta x^2 + O(\Delta x^2), \quad (21)$$

where

$$\phi_1 = 16(4 - \kappa)c, \quad (22)$$

$$\phi_2 = \frac{4}{3}(2 - \kappa)B'_{L,L}. \quad (23)$$

Note that the first-order term decays rapidly with the separation distance and becomes zero in the case of $c = 0$, whereas the other part of the error turns out to be second order in Δx.

Accordingly, the results are in line with the classical analysis again.

Let us study now the second-order error term. This term is a function of the separation distance r, the basic functions $A_{1,2}(r), C_{1,\ldots,5}(r), E_{1,2}(r)$, and their derivatives up to second order. The function is quite complicated; therefore, we specify here only the most relevant part, which includes the function $C_1(r)$. The error associated with $C_1(r)$ can be written as

$$\Upsilon = \varpi(\kappa + 2)r_\alpha r_\beta[(\kappa + 1)C_1 + 2rC'_1 + r^2 C''_1], \quad (24)$$

where $\varpi = 4/9$ and $\varpi = 4$ for D2Q9 and D3Q19 models, respectively.

One can see that this part of the error is strongly dependent on the separation distance, and one may presume that at large separation distance the error can become relevant as far as the derivatives of $C_1(r)$ are not negligible.

This result suggests that correlations obtained by lattice Boltzmann simulations should be considered with some caution, because the correlations can be distorted systematically at large separation distances by the numerical errors. Although one may expect that the above-mentioned errors are not relevant, it is worth making a grid refinement to check the results when correlations (or spectra) obtained by lattice Boltzmann simulations are studied.

V. THE INFLUENCE OF THE NONEQUILIBRIUM DISTRIBUTIONS

In order to study the influence of the nonequilibrium distribution functions on the correlations, we rewrite the evolution equation as follows:

$$f_i(\mathbf{x},t) = \left(1 - \frac{1}{\tau}\right)f_i(\mathbf{x} - \mathbf{c}_i\Delta x, t - \Delta t) + \frac{1}{\tau}f_i^{eq}(\mathbf{x} - \mathbf{c}_i\Delta x, t - \Delta t).$$

Now, the pressure can be obtained by

$$p(\mathbf{x},t) = \left(1 - \frac{1}{\tau}\right)\sum_i f_i(\mathbf{x} - \mathbf{c}_i\Delta x, t - \Delta t) + \frac{1}{\tau}\sum_i f_i^{eq}(\mathbf{x} - \mathbf{c}_i\Delta x, t - \Delta t).$$

In statistical steady state, the two-point pressure correlation can be written as follows:

$$\tilde{B}_{p,p}(\mathbf{r}) = \frac{1}{\tau^2}\tilde{B}^{eq}_{p,p}(\mathbf{r}) + \tilde{B}^{neq}_{p,p}(\mathbf{r}), \quad (25)$$

where

$$\tilde{B}^{eq}_{p,p}(\mathbf{r}) = \sum_{i,j}\langle f_i^{eq}(\mathbf{x} - \mathbf{c}_i\Delta x)f_j^{eq}(\mathbf{x} + \mathbf{r} - \mathbf{c}_j\Delta x)\rangle = \sum_{i,j}B^{eq}_{ij}(\mathbf{R}_{ij}),$$

and the nonequilibrium contribution is given by

$$\tilde{B}^{neq}_{p,p}(\mathbf{r}) = \frac{1}{\tau}\left(1 - \frac{1}{\tau}\right)[G_1(\mathbf{R}_{ij}) + G_2(\mathbf{R}_{ij})] + \left(1 - \frac{1}{\tau}\right)^2 G_3(\mathbf{R}_{ij}),$$

where

$$G_1(\mathbf{R}_{ij}) = \sum_{i,j}\langle f_i(\mathbf{x} - \mathbf{c}_i\Delta x)f_j^{eq}(\mathbf{x} + \mathbf{r} - \mathbf{c}_j\Delta x)\rangle,$$

$$G_2(\mathbf{R}_{ij}) = \sum_{i,j}\langle f_i^{eq}(\mathbf{x} - \mathbf{c}_i\Delta x)f_j(\mathbf{x} + \mathbf{r} - \mathbf{c}_j\Delta x)\rangle,$$

$$G_3(\mathbf{R}_{ij}) = \sum_{i,j}\langle f_i(\mathbf{x} - \mathbf{c}_i\Delta x)f_j(\mathbf{x} + \mathbf{r} - \mathbf{c}_j\Delta x)\rangle. \quad (26)$$

By performing a Chapman-Enskog expansion one can go a step further. So, we introduce the following expansions:

$$f_i(\mathbf{x} + \mathbf{c}_i\Delta x, t + \Delta t) = \sum_{i=0}^{\infty}\frac{\varepsilon^n}{n!}D^n_{t_n}f_i(\mathbf{x},t),$$

$$f_i = \sum_{n=0}^{\infty}\varepsilon^n f_i^{(n)}, \quad (27)$$

$$\partial_t = \sum_{n=0}^{\infty}\varepsilon^n\partial_{t_n}, \quad (28)$$

where $\varepsilon = \Delta x = \Delta t$ is a small parameter (the Knudsen number) and $D_{t_n} \equiv (\partial_{t_n} + c_{i\alpha}\partial_\alpha)$.

After some algebra, one can derive the following relations in the consecutive order of the small parameter [12]:

$$O(\varepsilon^0): \quad f_i^{(0)} = f_i^{eq}(x,t),$$

$$O(\varepsilon^1): -\frac{1}{\tau}f_i^{(1)} = D_{t_0}f_i^{(0)}, \tag{29}$$

and correspondingly we also can decompose the distribution functions as follows:

$$f_i = f_i^{eq} + \varepsilon f_i^{neq}, \tag{30}$$

where

$$f_i^{neq} = f_i^{(1)} + \varepsilon f_i^{(2)} + \cdots .$$

Substituting Eq. (30) into (26) yields

$$G_1(\mathbf{R}_{ij}) = \widetilde{B}_{p,p}^{eq}(\mathbf{R}_{ij}) + \varepsilon \sum_{i,j} B_{ij}^{neq,eq}(\mathbf{R}_{ij}),$$

$$G_2(\mathbf{R}_{ij}) = \widetilde{B}_{p,p}^{eq}(\mathbf{R}_{ij}) + \varepsilon \sum_{i,j} B_{ij}^{eq,neq}(\mathbf{R}_{ij}),$$

$$G_3(\mathbf{R}_{ij}) = \widetilde{B}_{p,p}^{eq}(\mathbf{R}_{ij}) + \varepsilon \sum_{i,j} [B_{ij}^{neq,eq}(\mathbf{R}_{ij}) + B_{ij}^{eq,neq}(\mathbf{R}_{ij})] + \varepsilon^2 \sum_{i,j} B_{ij}^{neq,neq}(\mathbf{R}_{ij}),$$

where

$$B_{ij}^{neq,eq}(\mathbf{R}_{ij}) = \langle f_i^{neq}(\mathbf{x} - \mathbf{c}_i\Delta x) f_j^{eq}(\mathbf{x} + \mathbf{r} - \mathbf{c}_j\Delta x)\rangle,$$

$$B_{ij}^{eq,neq}(\mathbf{R}_{ij}) = \langle f_i^{eq}(\mathbf{x} - \mathbf{c}_i\Delta x) f_j^{neq}(\mathbf{x} + \mathbf{r} - \mathbf{c}_j\Delta x)\rangle,$$

$$B_{ij}^{neq,neq}(\mathbf{R}_{ij}) = \langle f_i^{neq}(\mathbf{x} - \mathbf{c}_i\Delta x) f_j^{neq}(\mathbf{x} + \mathbf{r} - \mathbf{c}_j\Delta x)\rangle.$$

Collecting terms with the same order, the nonequilibrium contribution can be written as follows:

$$\widetilde{B}_{p,p}^{neq}(\mathbf{r}) = \left[\frac{2}{\tau}\left(1 - \frac{1}{\tau}\right) + \left(1 - \frac{1}{\tau}\right)^2\right]\widetilde{B}_{p,p}^{eq}(\mathbf{R}_{ij}) + \varepsilon\frac{2}{\tau}\left(1 - \frac{1}{\tau}\right) \times \left[\sum_{i,j}[B_{ij}^{neq,eq}(\mathbf{R}_{ij}) + B_{ij}^{eq,neq}(\mathbf{R}_{ij})]\right] \tag{31}$$

$$+ \varepsilon^2\left(1 - \frac{1}{\tau}\right)^2 \sum_{i,j} B_{ij}^{neq,neq}(\mathbf{R}_{ij}). \tag{32}$$

Substituting the nonequilibrium contribution (31) into (25), one obtains the lattice Boltzmann pressure correlation for arbitrary relaxation time

$$\widetilde{B}_{p,p}(\mathbf{r}) = \widetilde{B}_{p,p}^{eq}(\mathbf{R}_{ij}) + \varepsilon\frac{2}{\tau}\left(1 - \frac{1}{\tau}\right)\left[\sum_{i,j}[B_{ij}^{neq,eq}(\mathbf{R}_{ij}) + B_{ij}^{eq,neq}(\mathbf{R}_{ij})]\right] + \varepsilon^2\left(1 - \frac{1}{\tau}\right)^2\sum_{i,j} B_{ij}^{neq,neq}(\mathbf{R}_{ij}).$$

Obviously, in the case of $\tau=1$ we get back the results obtained in the previous sections, but in any other case the nonequilibrium distributions influence the correlation functions through their correlation with the equilibrium (first-order effect) and the nonequilibrium distributions (second-order effect).

Using the second relation of (29), one can express the nonequilibrium in terms of equilibrium distributions, that is by macroscopic quantities, and the nonequilibrium contribution can be given explicitly. However, the expression obtained in such way is far more complicated than the expression obtained for the equilibrium correlation, and it does not suggest a simple interpretation. Therefore, numerical experiments are planned to be performed in order to obtain further information about the nonequilibrium contribution.

It is worth mentioning that one can apply diffusive scaling instead of the classical one used in this section. It has been demonstrated in Ref. [15] that the diffusive scaling and the application of a LBM equivalent moment system can yield directly the incompressible Navier-Stokes equations instead of the compressible one. Such treatment may have the advantage of a simpler derivation, and further simplifications in the results might be obtained.

VI. CONCLUSION

Analytical results habe been derived for the two-point pressure and velocity correlations in the case of steady, homogeneous, isotropic turbulence based on the lattice Boltzmann equation. It has been shown that both the pressure and the velocity correlations have first-order deviation terms due to the finite lattice spacing. In the low Mach number limit, the first-order terms disappear.

However, the second-order error is a weighted combination of two-point correlation functions and their derivatives. Accordingly, the error can behave systematically. Because the weights are powers of the separation distance, they may become relevant at large separation distances. Therefore, it is worth checking the lattice Boltzmann simulation results by grid refinement when details of the correlations (or spectra) are studied.

The two-point correlations between pressure and velocity are in direct relation to the two-point correlations between the equilibrium distributions in lattice Boltzmann models. The nonequilibrium distributions give further first- and second-order contributions to those correlations.

The situation considered in this paper starts from "macroscopically ideal" fields, i.e., the pressure and velocity fields are homogeneous and isotropic. Numerical experiments need to be performed in order to study nonideal problems and to clarify the effect of the nonequilibrium distributions.

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