Comment on "Alternative approach to the solution of the dispersion relation for a generalized lattice Boltzmann equation"

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(Received 26 February 2008; published 11 December 2008)

Recently Reis and Phillips [Phys. Rev. E **77**, 026702 (2008)] proposed a perturbative method to solve the dispersion equation derived from the linearized lattice Boltzmann equation. We will demonstrate that the method proposed by Reis and Phillips is a reinvention of an existing method. We would also like to refute a number of claims made by Reis and Phillips.

DOI: 10.1103/PhysRevE.78.068701 PACS number(s): 47.11.−j

In a recent article [1], Reis and Phillips (RP) propose a "more elegant and transparent" approach based on perturbation analysis to solve the "difficult dispersion problem" derived from the linearized lattice Boltzmann equation (LBE), as an alternative to the approach of Lallemand and Luo (LL) [2]. The reasons for their alternative, as RP argue, are that the approach of LL is "lacking rigor" and "unjustified," "in particular when the Knudsen number is large." RP further claim that (i) their "derived transport coefficients are valid for all Knudsen numbers" and (ii) their "perturbative analysis obviates the need to perform a Chapman-Enskog analysis." The purpose of this Comment is to demonstrate that, first, the "alternative" of RP is a reinvention of an existing method [3–5], and second, the above claims made by RP are false.

The LBE can be written concisely in a vector form

$$\mathbf{f}(\boldsymbol{x}_j + \boldsymbol{c}\,\delta_t, t_n + \delta_t) - \mathbf{f}(\boldsymbol{x}_j, t_n) = \boldsymbol{\Omega}(\boldsymbol{x}_j, t_n), \tag{1}$$

where bold-font symbols denote Q-tuple vectors for an LBE model with Q discrete velocities $\{\mathbf{c}_i | i=0,1,\ldots,b\}$, $b=(Q-1)$:

$$\mathbf{f}(\boldsymbol{x}_j, t_n) \coloneqq (f_0(\boldsymbol{x}_j, t_n), f_1(\boldsymbol{x}_j, t_n), \ldots, f_b(\boldsymbol{x}_j, t_n))^\dagger,$$

$$\mathbf{f}(\boldsymbol{x}_j + \boldsymbol{c}\,\delta_t, t_n + \delta_t) \coloneqq (f_0(\boldsymbol{x}_j, t_n + \delta_t),$$

$$f_1(\boldsymbol{x}_j + \boldsymbol{c}_1\delta_t, t_n + \delta_t), \ldots, f_b(\boldsymbol{x}_j + \boldsymbol{c}_b\delta_t, t_n + \delta_t))^\dagger,$$

$$\boldsymbol{\Omega}(\boldsymbol{x}_j, t_n) \coloneqq (\Omega_0(\boldsymbol{x}_j, t_n), \Omega_1(\boldsymbol{x}_j, t_n), \ldots, \Omega_b(\boldsymbol{x}_j, t_n))^\dagger,$$

where † denotes transpose operation; that is, $\mathbf{f}(\boldsymbol{x}_j, t_n)$ is the vector of precollision values of $\{f_i\}$ at a lattice node $\boldsymbol{x}_j$, $\mathbf{f}(\boldsymbol{x}_j + \boldsymbol{c}\,\delta_t, t_n + \delta_t)$ is the vector of the post-collision values of $\{f_i\}$ which have been transported to the nodes about $\boldsymbol{x}_j$ according to the discrete velocity set $\{\boldsymbol{c}_i\}$, and $\Omega(\mathbf{x}_j, t_n)$ is the vector of the changes due to collision. Obviously, one cannot expect to obtain analytic solutions of Eq. (1) in general. As usual we have to deal with the linearization of Eq. (1):

$$\delta\mathbf{f}(\boldsymbol{x}_j + \boldsymbol{c}\,\delta_t, t_n + \delta_t) - \delta\mathbf{f}(\boldsymbol{x}_j, t_n) = \mathsf{J} \cdot \delta\mathbf{f}(\boldsymbol{x}_j, t_n), \tag{2}$$

where $\delta\mathbf{f} \coloneqq \mathbf{f} - \mathbf{f}^{(0)}$, $\mathbf{f}^{(0)}$ is the vector of equilibria of $\{f_i\}$, J is the Jacobian,

$$\mathsf{J} \coloneqq \frac{\partial \boldsymbol{\Omega}}{\partial \mathbf{f}}(\mathbf{f} = \mathbf{f}^{(0)}), \tag{3}$$

and $\boldsymbol{\Omega}(\mathbf{f}^{(0)}) = 0$. The spatial Fourier transform of Eq. (2) is

$$\mathsf{D}^{-1} \cdot \delta\tilde{\mathbf{f}}(\boldsymbol{k}_m, t_n + \delta_t) - \delta\tilde{\mathbf{f}}(\boldsymbol{k}_m, t_n) = \mathsf{J} \cdot \delta\tilde{\mathbf{f}}(\boldsymbol{k}_m, t_n), \tag{4}$$

where $\delta\tilde{\mathbf{f}}(\boldsymbol{k}_m, t_n)$ is the (discrete) Fourier transform of $\delta\mathbf{f}(\boldsymbol{x}_j, t_n)$, D^{-1} is the advection operator, and D is a $Q \times Q$ diagonal matrix with the following elements:

$$D_{ij} \coloneqq e^{-\imath \boldsymbol{c}_i \cdot \boldsymbol{k}_m \delta_t} \delta_{ij},$$

where $\imath \coloneqq \sqrt{-1}$. Equation (4) can be concisely written as

$$\delta\tilde{\mathbf{f}}(\boldsymbol{k}_m, t_n) = \mathsf{H}^n \cdot \delta\tilde{\mathbf{f}}(\boldsymbol{k}_m, t_0), \tag{5}$$

where the linearized evolution operator H is

$$\mathsf{H} \coloneqq \mathsf{D} \cdot (\mathsf{I} + \mathsf{J}),$$

and I is the $Q \times Q$ identity matrix. The solution of the linearized LBE (2) is equivalent to the eigenvalue problem of H, which cannot be solved analytically in general. A perturbative approach by expanding D in powers of δ_t (or $\boldsymbol{k}_m$) is used to solve the eigenvalue problem [3–5]:

$$\mathsf{D} = \sum_{n=0}^{\infty} \frac{1}{n!} \delta_t^n \mathsf{K}^n, \tag{6}$$

where the elements of the diagonal matrix K are

$$K_{ij} = -\imath \boldsymbol{c}_i \cdot \boldsymbol{k}_m \delta_{ij}.$$

Hence H is also expanded in powers of δ_t:

$$\mathsf{H} = \sum_{n=0}^{\infty} \frac{1}{n!} \delta_t^n \mathsf{H}^{(n)}, \quad \mathsf{H}^{(n)} \coloneqq \mathsf{K}^n(\mathsf{I} + \mathsf{J}). \tag{7}$$

The perturbative solution for the eigenvalue problem of H can be obtained order by order in $\boldsymbol{k}_m$ in the space spanned by the eigenvectors of $\mathsf{H}^{(0)} = (\mathsf{I} + \mathsf{J})$, which can be constructed in several ways [2–4]. This perturbative method in RP is indeed

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identical to the existing method formulated by Luo *et al.* to compute the transport coefficients from the linearized LBE [3–5]. The only difference, as far as we can tell, is in the specifics of J: the Jacobian J in the early work of Luo *et al.* [3–5] is derived from various lattice gas automaton (LGA) models, while that in RP is the one derived from the multiple-relaxation-times (MRT) LBE given by LL [2]. In other words, RP apply the technique developed earlier by Luo *et al.* [3–5] to the generalized LBE model studied by LL [2] and obtain results identical to those given by LL [2]; not a single new result was given by RP.

In LL [2], the Gaussian elimination was used to obtain a $(d+1)\times(d+1)$ matrix for $d+1$ conserved modes in d dimensions from a $Q\times Q$ matrix for athermal LBE models of Q velocities. The eigenvalue problem is solved perturbatively in terms of the relaxation rates $\{s_i\}$. This is a formal approach, and the reason one can neglect terms related to certain relaxation rates is because of separation of scales related to these modes. The argument of scale separation has its physical basis and can be justified rigorously in the asymptotic limit [6]. The calculations of the eigenvalues of the matrix H as functions of $\boldsymbol{k}$ can be systematically carried out by computer algebra software such as Mathematica or Maple. The fact that the perturbation method of Luo *et al.* [3–5] used by RP and the Gaussian elimination used by LL yield identical results indicate that these two methods are identical. RP's argument that LL's approach is "lacking rigor" and "unjustified" is thus unfounded.

The work of RP did not only reinvent an existing method and repeat existing results, but contains erroneous claims which will be addressed in the following. RP repeatedly claim that their "derived transport coefficients are valid for all Knudsen numbers." First of all, we should point out that in the diffusive limit of $\delta_x^2=\delta_t\rightarrow 0$ for incompressible flows, the LBE does not converge to the Boltzmann equation [6]; consequently, it cannot correctly model severe nonequilibrium effects due to finite Knudsen numbers. Second, to correctly model slip flows, various slip-velocity models must be *explicitly* incorporated into the LBE [7]. The velocity profile obtained from various LBE models for a microchannel is a *linear* superposition of a *perfect* parabola and a "slip" at the boundary [5,8]. It is clear that the LBE in its present form cannot possibly capture the Knudsen layer, regardless the number of discrete velocities (e.g., [8,9]). Evidence shows that the lattice BGK models referred to by RP reproduce qualitatively incorrect results with a moderate Knudsen number $\mathrm{Kn}=0.388$ for a long microchannel [7,10]. Solutions of a simple *linearized* LBE could not possibly have anything to do with the Knudsen effect in rarefied gases. Finally, when Kn is large, the flow is far from equilibrium which implies that a macroscopic theory and subsequently the concept of transport coefficients are no longer valid. Thus the transport coefficients derived by RP can definitively not be "valid for all Knudsen numbers."

In addition, RP repeatedly state that the analysis of the linearized dispersion equation (LDE) can make the Chapman-Enskog analysis "redundant." This is false. For instance, the LDE analysis cannot retrieve the nonlinear advection term $\boldsymbol{u}\cdot\boldsymbol{\nabla u}$ in the Navier-Stokes equation; it cannot be used to analyze the effects due to boundary conditions (e.g., [11]), and for non-Newtonian fluids, it cannot yield nonlinear terms involving products of $\boldsymbol{j}:=\rho\boldsymbol{u}$, $\boldsymbol{\nabla u}$ and other higher-order derivatives of hydrodynamic variables which are important for viscoelastic fluids [12]. The usefulness of the LDE lies in its ability to analyze the numerical artifacts due to finite grid size δ_x. However, the Chapman-Enskog analysis has to deal with both δ_x and δ_t, and the difficulty of circumventing the Chapman-Enskog analysis is not coming from a finite δ_x, but from a finite δ_t.

Finally, RP characterized the LBE with the MRT collision model as "simply a refined, and renamed, version of the quasilinear LBE of Higuera and Jimenez." This is inaccurate and misleading. It was D. d'Humières who first formulated the MRT LBE in its present form [13]. That is, the advection is executed in velocity space $\mathbb{V}=\mathbb{R}^Q$, while the collision is carried out in moment space $\mathbb{M}=\mathbb{R}^Q$, and this projection from velocity space $\mathbb{V}$ to moment space $\mathbb{M}$ is absent in the linear LBE of Higuera and Jiménez [14]. We would like to emphasize that this projection from velocity space $\mathbb{V}$ to moment space $\mathbb{M}$ is essential and crucial for *efficient* implementation of LBE algorithms [15], and it can be related to Grad's theory [16] and mode-mode analysis. We would also like to note that the MRT LBE has also been developed by others independently. McNamara *et al.* used the MRT LBE in a series of papers on thermal hydrodynamics [17–19]. Following McNamara *et al.*, Ladd used the MRT LBE for simulations of particulate suspensions [20,21]. While these authors have contributed to the development of the MRT-LBE method [17–21], their emphasis was more on the application rather than the methodology *per se*. The work of d'Humières [13] was the first systematic theoretical formulation of the MRT-LBE method in its full extend.

In conclusion, the perturbative method used by RP is a reinvention of an existing method [3–5] and the paper of RP contains no new result. In addition, the claims made by RP concerning the ability of the LBE to model finite-Knudsen-number effects and that of the LDE analysis to circumvent the Chapman-Enskog analysis are false.

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