Non-hydrodynamic modes and general equations of state in lattice Boltzmann equations

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The lattice Boltzmann equation is commonly used to simulate fluids with isothermal equations of state in a weakly compressible limit, and intended to approximate solutions of the incompressible Navier–Stokes equations. Due to symmetry requirements there are usually more degrees of freedom in the equilibrium distributions than there are constraints imposed by the need to recover the Navier–Stokes equations in a slowly varying limit. We construct equilibria for general barotropic fluids, where pressure depends only upon density, using the two dimensional, nine velocity (D2Q9) and one dimensional, five velocity (D1Q5) lattices, showing that one otherwise arbitrary function in the equilibria must be chosen to suppress instability.

Keywords: lattice Boltzmann, barotropic fluids, eigenvalues, stability, non-hydrodynamic variables

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I. INTRODUCTION

Methods based on the lattice Boltzmann equation (LBE) have become very popular for simulating fluid flow [1–3]. Most common LBEs are used to approximate incompressible flows, using an isothermal equation of state with sound speed much larger than the maximum speed of fluid flow. The LBE is much less well developed for simulating fluids with other equations of state, such as the van der Waals or Enskog equations describing dense gases, or the shallow water equations from geophysical fluid dynamics.

An LBE is an evolution equation for a set of distribution functions $f_i(\mathbf{x}, t)$ that specify the densities of particles at position $\mathbf{x}$ moving with velocity $\boldsymbol{\xi}_i$,

$$\partial_t f_i + \boldsymbol{\xi}_i \cdot \nabla f_i = -\frac{1}{\tau}(f_i - f_i^{(0)}). \tag{1}$$

Macroscopic variables like fluid density ρ, momentum $\rho\mathbf{u}$, and momentum flux $\mathbf{\Pi}$, are expressed as moments of the f_i,

$$\rho = \sum_i f_i, \quad \rho\mathbf{u} = \sum_i \boldsymbol{\xi}_i f_i, \quad \mathbf{\Pi} = \sum_i \boldsymbol{\xi}_i\boldsymbol{\xi}_i f_i, \quad \mathbf{\Pi}^{(0)} = \sum_i \boldsymbol{\xi}_i\boldsymbol{\xi}_i f_i^{(0)}, \tag{2}$$

discrete analogs of the integral moments from continuum kinetic theory.

The Bhatnagar–Gross–Krook or BGK collision operator on the right hand side of (1) relaxes the f_i towards a specified equilibrium $f_i^{(0)}$ with a single timescale τ. The $f_i^{(0)}$ are functions of ρ and $\mathbf{u}$, chosen in such a way that mass and momentum are conserved by collisions. In this paper we consider only barotropic fluids so there is no separate internal energy. The zeroth and first moments of (1) then yield the macroscopic conservation laws

$$\partial_t\rho + \nabla\cdot(\rho\mathbf{u}) = 0, \quad \partial_t(\rho\mathbf{u}) + \nabla\cdot\mathbf{\Pi} = 0. \tag{3}$$

An equation for the momentum flux $\mathbf{\Pi}$ may be obtained from the second ($\boldsymbol{\xi}_i\boldsymbol{\xi}_i$) moment of equation (1),

$$\partial_t\mathbf{\Pi} + \nabla\cdot\left(\sum_i \boldsymbol{\xi}_i\boldsymbol{\xi}_i\boldsymbol{\xi}_i f_i\right) = -\frac{1}{\tau}\left(\mathbf{\Pi} - \mathbf{\Pi}^{(0)}\right), \tag{4}$$

using the Chapman–Enskog expansion for small τ and $f_i = f_i^{(0)} + O(\tau)$. This corresponds to seeking solutions that vary slowly on the timescale set by τ.

Determining suitable $f_i^{(0)}$ for which (3) and (4) yield the desired Navier–Stokes equations is usually the most challenging part of constructing a viable LBE. The leading order (Euler) hydrodynamic equations imply the constraints

$$\sum_i f_i^{(0)} = \rho, \quad \sum_i \boldsymbol{\xi}_i f_i = \rho\mathbf{u}, \quad \sum_i \boldsymbol{\xi}_i\boldsymbol{\xi}_i f_i^{(0)} = \mathbf{\Pi}^{(0)} = P(\rho) + \rho\mathbf{u}\mathbf{u}, \tag{5}$$

where $P(\rho)$ is the pressure for a barotropic fluid. Obtaining a correct viscous stress from (4) implies further constraints on $\sum_i \boldsymbol{\xi}_i\boldsymbol{\xi}_i\boldsymbol{\xi}_i f_i$.

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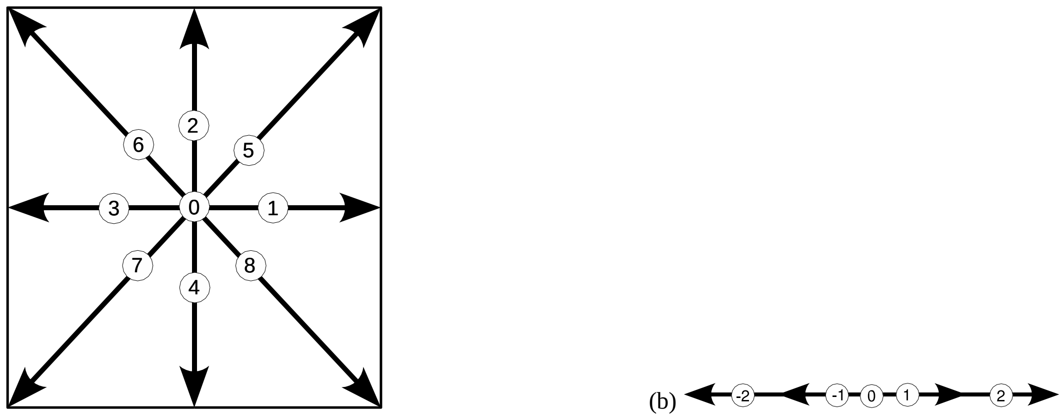
FIG. 1: Arrangement of velocity vectors $\boldsymbol{\xi}_i$ for (a) the two dimensional, nine velocity (D2Q9) lattice, and (b) the one dimensional, five velocity (D1Q5) lattice.

(a)



However, these constraints generally do not suffice to determine the $f_i^{(0)}$ uniquely. For example, (5) provides six independent constraints in two dimensions, yet one typically uses a square lattice with nine velocities, or nine degrees of freedom, as shown in figure 1(a). For this lattice (4) implies only two further constraints, leaving one degree of freedom undetermined [4].

Moreover, the resulting equilibria should lead to a stable numerical scheme when (1) is discretised as

$$\overline{f}_i(\mathbf{x}+\boldsymbol{\xi}_i\Delta t, t+\Delta t) - \overline{f}_i(\mathbf{x},t) = -\frac{\Delta t}{\tau+\Delta t/2}\left[\overline{f}_i(\mathbf{x},t) - f_i^{(0)}(\mathbf{x},t)\right]. \tag{6}$$

The $\overline{f}_i$ are related to the previous f_i by $\overline{f}_i = f_i + (f_i - f_i^{(0)})\Delta t/(2\tau)$. This change of variables renders (6) a second order accurate approximation to the PDE (1), at the price of becoming prone to instabilities when $\tau \ll \Delta t$. Although this regime gives high grid-scale Reynolds numbers, the factor before the $[\cdots]$ term in (6) becomes close to -1, so the $\overline{f}_i$ are highly *over-relaxed* at each timestep.

Any resulting instabilities that arise on the grid scale are not visible to the slowly varying Chapman–Enskog expansion, so an alternative approach must be developed. We first review Dellar's work [4] for the D2Q9 lattice, showing that the usual expansion as polynomials in the particle velocities $\boldsymbol{\xi}_i$ leads to instability for any equation of state except the usual $P = \frac{1}{3}\rho$ in lattice units ($\Delta x = \Delta t = 1$), but that stability may be restored by suitable choice of a non-hydrodynamic or "ghost" component of the equilibrium. We then obtain analogous results for the D1Q5 lattice shown in figure 1(b).

II. BAROTROPIC FLOWS WITH THE D2Q9 LATTICE

The most commonly used lattice is probably the two dimensional, nine velocity (D2Q9) lattice shown in figure 1(a), with the equilibria [5]

$$f_i^{(0)} = w_i\left[\rho 1_i + 3(\rho\mathbf{u})\cdot\boldsymbol{\xi}_i + \frac{9}{2}(\rho\mathbf{u}\mathbf{u}) : (\boldsymbol{\xi}_i\boldsymbol{\xi}_i - \frac{1}{3}\mathsf{I})\right], \tag{7}$$

with weights w_i given by

$$w_0 = 4/9, \quad w_{1,2,3,4} = 1/9, \quad w_{5,6,7,8} = 1/36. \tag{8}$$

These equilibria give an isothermal equation of state with $P = \frac{1}{3}\rho$ in lattice units ($\Delta x = \Delta t = 1$).

The three terms in (10) correspond to an expansion in the tensor Hermite polynomials 1, $\boldsymbol{\xi}$, $(\boldsymbol{\xi}\boldsymbol{\xi} - \frac{1}{3}\mathsf{I})$. These polynomials are orthogonal with respect to the weighted inner product $\langle f, g\rangle = \sum_i w_i f_i g_i$, and also with respect to the continuous inner product with Gaussian weight factor $\exp(-3|\boldsymbol{\xi}|^2/2)$. He & Luo [6] used this fact to rederive (7) from the continuum Maxwell–Boltzmann equilibrium distribution by Gaussian quadrature in their *"a priori"* approach.

However, these tensor Hermite polynomials control only six of the nine degrees of freedom in the D2Q9 equilibria. They may be completed to form an orthogonal basis for $\mathbb{R}^9$ using the vectors $g_i = (1, -2, -2, -2, -2, 4, 4, 4, 4)^{\mathsf{T}}$ and $g_i\boldsymbol{\xi}_i$. By analogy with the hydrodynamic variables ρ, $\rho\mathbf{u}$, $\boldsymbol{\Pi}$ defined in (2), we define non-hydrodynamic or "ghost" [3] variables N and $\mathbf{J}$ by the moments

$$N = \sum_i g_i f_i, \quad \mathbf{J} = \sum_i g_i\boldsymbol{\xi}_i f_i, \quad N^{(0)} = \sum_i g_i f_i^{(0)}, \quad \mathbf{J}^{(0)} = \sum_i g_i\boldsymbol{\xi}_i f_i^{(0)}, \tag{9}$$

(see also Ref. [7]). A general set of equilibria may thus be written as [4]

$$f_i^{(0)} = w_i\left[\rho 1_i + 3(\rho\mathbf{u})\cdot\boldsymbol{\xi}_i + \frac{9}{2}(\boldsymbol{\Pi}^{(0)} - \frac{1}{3}\rho\mathsf{I}) : (\boldsymbol{\xi}_i\boldsymbol{\xi}_i - \frac{1}{3}\mathsf{I}) + \frac{1}{4}g_i N^{(0)} + \frac{3}{8}g_i\,\boldsymbol{\xi}_i\cdot\mathbf{J}^{(0)}\right], \tag{10}$$

where the previous equilibria coincide with just the first three terms of (10). However, the Euler equations are satisfied for any choice of $N^{(0)}$ and $\mathbf{J}^{(0)}$, not just $N^{(0)} = \mathbf{J}^{(0)} = 0$ as in the Hermite expansion. While $\mathbf{J}^{(0)}$ turns out to be constrained by the viscous stress, $N^{(0)}$ is left completely arbitrary [4].

To determine $N^{(0)}$, Dellar [4] derived a wave equation approximately describing short scale density perturbations,

$$\frac{\partial^2 \rho}{\partial t^2} = \nabla^2 P(\rho) + 2\tau^2 \frac{\partial^4 Q(\rho)}{\partial x^2 \partial y^2}, \text{ where } Q = P(\rho) - \frac{1}{3}\rho + \frac{1}{3}N^{(0)}, \tag{11}$$

assuming that $N^{(0)}$ depends only on ρ. The corresponding dispersion relation for linear waves of the form $\rho = \rho_0 + \rho' \exp(i\mathbf{k} \cdot \mathbf{x} + \sigma t)$ is

$$\sigma^2 = -(k_x^2 + k_y^2) \frac{dP}{d\rho}\Big|_{\rho=\rho_0} + 2\tau^2 k_x^2 k_y^2 \frac{dQ}{d\rho}\Big|_{\rho=\rho_0}. \tag{12}$$

The first term on the right hand side of (12) gives the expected sound waves with speed $c_{\rm s} = (dP/d\rho)^{1/2}$. However, the second term involving Q gives either ill-posed growth (when $dQ/d\rho > 0$) or very high frequency dispersive waves (when $dQ/d\rho < 0$). In both cases, the timescale is proportional to $|\mathbf{k}|^2$, rather than to $|\mathbf{k}|$ as for sound waves. It is easy to suppose that high frequency waves, with phase speed proportional to $|\mathbf{k}|$, would become unstable through violating the Courant–Friedrichs–Lewy (CFL) condition for the discrete system (6).

Stable equilibria for an arbitrary barotropic equation of state $P = P(\rho)$ are thus given by choosing $N^{(0)}$ to set $Q = 0$,

$$f_i = w_i \Big[\rho 1_i + 3(\rho \mathbf{u}) \cdot \boldsymbol{\xi}_i + \frac{9}{2}(\rho \mathbf{u}\mathbf{u} + P\mathsf{I} - \frac{1}{3}\rho \mathsf{I}) : (\boldsymbol{\xi}_i \boldsymbol{\xi}_i - \frac{1}{3}\mathsf{I}) + \frac{1}{4}(\rho - 3P) g_i \Big]. \tag{13}$$

They coincide with Salmon's [8] equilibria for the particular case $P = \frac{1}{2} g \rho^2$ that yields the shallow water equations. In general the g_i term means that they do not coincide with a truncation in tensor Hermite polynomials, or with a small Mach number expansion of the Maxwellian in continuum kinetic theory. The only exception is the special case $P = \frac{1}{3}\rho$ that sets the coefficient in the final term to zero, so (13) coincides with the usual isothermal equilibria (7).

III. BAROTROPIC FLOWS WITH THE D1Q5 LATTICE

We now derive similar equilibria for the D1Q5 lattice using the five velocities $\xi_i = i$ for $i = -2, -1, 0, 1, 2$ as sketched in figure 1(b). For this lattice Qian & Zhou [9] proposed the equilibria

$$f_i^{(0)} = w_i \big[\rho + \rho u \xi_i + \tfrac{1}{2} \rho u^2 (\xi_i^2 - 1) + \tfrac{1}{2} \rho u^3 (\xi_i^3 - 3\xi_i) \big], \tag{14}$$

with equation of state $P = \rho$, or dimensionless temperature $\theta = 1$. The weights are $w_0 = 1/2$, $w_{\pm 1} = 1/6$, and $w_{\pm 2} = 1/12$. The u^3 term eliminates an erroneous $\nabla \cdot (\rho \mathbf{uuu})$ contribution to the viscous stress, as in the D2Q9 equilibria [10].

The four lattice vectors 1_i, ξ_i, $\xi_i^2 - 1$ and $\xi_i^3 - 3\xi_i$ appearing in (14) are orthogonal with respect to a weighted inner product with the above weights. They may be completed by $g_i = (1, -2, 1, -2, 1) = \xi_i^4 - 4\xi_i^2 + 1$ to form an orthogonal basis for $\mathbb{R}^5$.

Equilibria yielding the one dimensional Euler equations with the barotropic equation of state $P = P(\rho)$ may thus be written as

$$f_i^{(0)} = w_i \big[\rho + \rho u \xi_i + \tfrac{1}{2} (P(\rho) - \rho + \rho u^2)(\xi_i^2 - 1) + \tfrac{1}{2} \rho u^3 (\xi_i^3 - 3\xi_i) + g_i N^{(0)} \big], \tag{15}$$

where again $N^{(0)}$ is an arbitrary function of ρ (at least) that is not determined by the Chapman–Enskog expansion, at either the Euler or Navier–Stokes orders. For $p = \rho$ and $N^{(0)} = 0$, the equilibria (15) coincide with those in (14).

The u^3 term plays no rôle in the following analysis, which is based on linearising around a rest state ($u = 0$). However, this term should really also involve the pressure to achieve a Galilean invariant viscous stress (see appendix)

It does not seem possible (see below) to derive a wave equation analogous to (11) characterising which functions $N^{(0)}$ give stable simulations. Instead, we consider solutions close to a global rest-state equilibrium,

$$\overline{f}_i(x_m, t) = f_i^{(0)}(\rho = 1, u = 0) + \epsilon h_i(x_m, t), \tag{16}$$

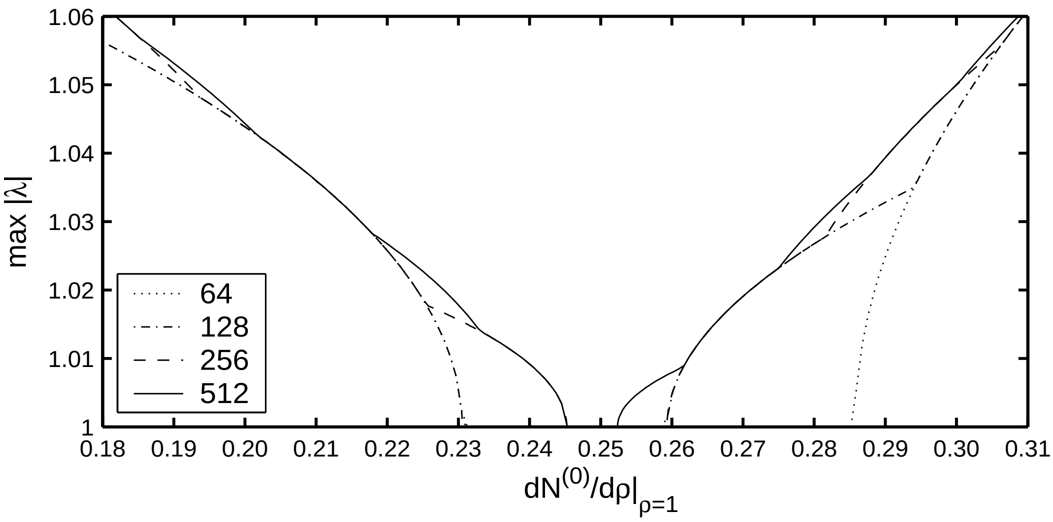
on a periodic domain with M equally spaced points $x_m = m\Delta x$. For $\epsilon \ll 1$, the h_i then evolve according to the linearised equation

$$h_i(x_m + \xi_i \Delta t, t + \Delta t) - h_i(x_m, t) = -\frac{\Delta t}{\tau + \Delta t/2} \Omega_{ij} h_j(x_m, t), \tag{17}$$

where the 5×5 matrix Ω_{ij} arises from linearising the dependence of $f_i^{(0)}$ on the f_i via ρ and u in the full BGK collision operator (6).

Equation (17) implicitly defines a $5M \times 5M$ matrix taking the complete set of values $\{h_i(x_m, t)\}$ at one timestep to their values $\{h_i(x_m, t + \Delta t)\}$ at the next timestep. Linear stability of the overall scheme is then determined by the eigenvalues $\lambda_1, \ldots, \lambda_{5M}$

FIG. 2: Maximum amplification factor for the eigenmodes as a function of $N^{(0)}$, for lattices with 64, 128, 256, and 512 points, and equation of state $P(\rho) = \frac{1}{2}\rho$.

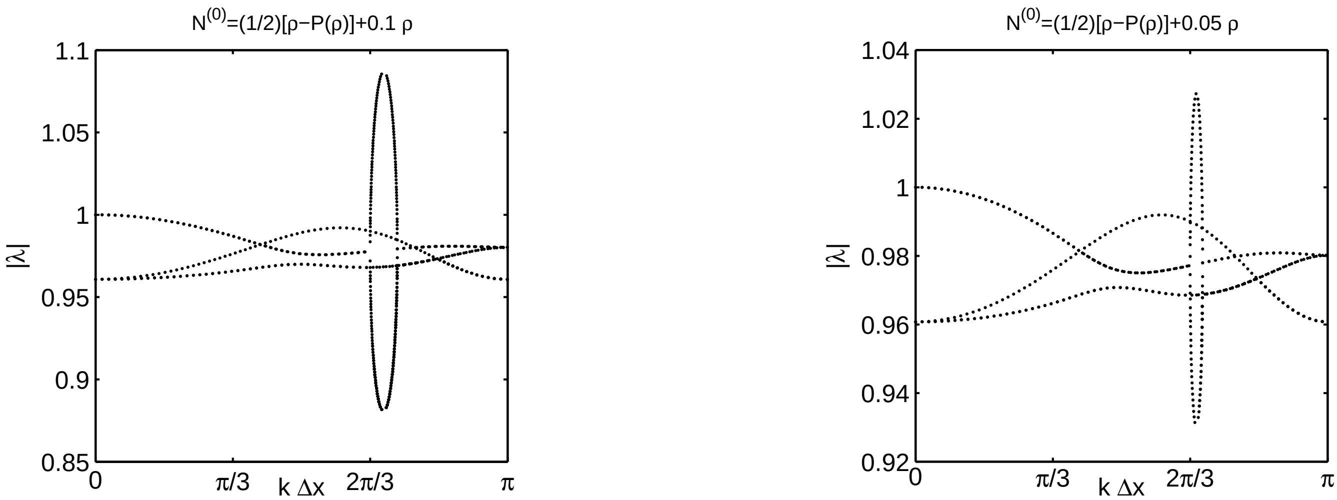


of this large matrix. More specifically, the scheme is stable when the moduli of the eigenvalues, or the amplification factors of the eigenmodes over a timestep, are all less than or equal to unity.

Figure 2 shows how the maximum modulus of the eigenvalues depends on the choice of function $N^{(0)}$ for equation of state $P(\rho) = \frac{1}{2}\rho$. In the linearised formulation (17) only the value $dN^{(0)}/d\rho|_{\rho=\rho_0}$ is relevant. The eigenvalues were computed using the QR algorithm implemented by the LAPACK routine DGEEV [11]. There are always neutrally stable modes, such as spatial translations by lattice spacings, so the maximum modulus is never less than one.

The scheme (6) is linearly stable ($\max|\lambda| = 1$) for quite a wide range of $N^{(0)}$ on a coarse lattice with 64 points. However, this stability window shrinks for finer lattices that support additional modes, allowing more scope for instability, until one is forced to choose $N^{(0)} = \frac{1}{4}\rho$. Similar computations for other equations of state lead to the conclusion that one must choose $N^{(0)} = \frac{1}{2}[\rho - P(\rho)]$ for stability, although, as before, all choices of $N^{(0)}$ lead to the same hydrodynamic equations from the Chapman–Enskog expansion at Navier–Stokes order.

FIG. 3: Amplication factors of Fourier modes for $P = \frac{1}{2}\rho$, $\tau = 0.01$, and two unstable choices of $N^{(0)}$. Instability is confined to a band of wavenumbers $k\Delta x \gtrsim 2\pi/3$.



IV. CONCLUSION

Obtaining correct hydrodynamics from the Chapman–Enskog expansion imposes constraints on the first few moments of the discrete equilibria $f_i^{(0)}$ in a lattice Boltzmann equation. Generally these constraints fail to determine unique equilibria, since the lattice contains more degrees of freedom (as may be required to ensure isotropy) than there are constraints. Following an earlier approach [4] for the D2Q9 lattice, we have found stable equilibria for the D1Q5 lattice reproducing arbitrary barotropic equations of state. A nonhydrodynamic variable $N^{(0)}$ that is not constrained by the Chapman–Enskog expansion must be chosen as $N^{(0)} = \frac{1}{2}[\rho - P(\rho)]$ to suppress instabilities.

We did this by examining the linear stability of all possible modes on a given sized lattice, as plotted in figure 2, and found windows of stable $N^{(0)}$ that shrank as the lattice was refined. Alternatively, we may consider only the stability of Fourier modes with some wavenumber k, equivalent to setting $h_i(x_m, t) \propto \exp(ikx_m)$ in (17). Figure 3 shows the amplification factors as functions of k for all 5 such modes, for two different unstable choices of $N^{(0)}$.

The unstable modes with $|\lambda| > 1$ do not extend back to small k, unlike the D2Q9 case shown in figures 4 and 5 of Ref. [4], even for larger values of τ than used here. Instability is confined to a small band of finite wavenumbers $k\Delta x \gtrsim 2\pi/3$. This suggests that a PDE approach like (11), being essentially a long wave analysis, albeit pursued to higher order than the Chapman–Enskog expansion, cannot be applied to determine stability on the D1Q5 lattice. Instead one must solve numerical eigenvalue problems, either for a whole lattice in one go as in figure 2, or wavenumber by wavenumber as in figure 3. Although the latter approach may be computationally cheaper, since the QR algorithm's cost grows as M^3 for an $M \times M$ matrix, it is easy to miss unstable modes, especially when they are confined to narrow bands as in this example. Moreover these bands's widths shrink to zero as one approaches the stable choice of $N^{(0)}$.

Finally, in principle $N^{(0)}$ may depend on all the f_i individually, not just on $\rho = \sum_i f_i$ as assumed here, which may offer further gains in stability.

V. ACKNOWLEDGMENTS

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APPENDIX A: EQUILIBRIA GIVING A GALILEAN-INVARIANT VISCOUS STRESS

The equilibria in (15) have the shortcoming that the viscous stress is not correctly Galilean invariant. It contains terms involving the density gradient like those coming from the equilibria (13) when $P \neq \frac{1}{3}\rho$ [4, 8].

Changing the coefficient of the ξ_i^3 term to $\rho u^3 + 3(P - \rho)u$,

$$\begin{aligned} f_i^{(0)} = w_i\big[\rho + \rho u\xi_i \;&+\; \tfrac{1}{2}(P(\rho) - \rho + \rho u^2)(\xi_i^2 - 1) \\ &+\; \tfrac{1}{2}[\rho u^3 + 3(P(\rho) - \rho)u](\xi_i^3 - 3\xi_i) + g_i N^{(0)}\big], \end{aligned} \tag{A1}$$

one obtains the Galilean-invariant viscous stress

$$\Pi^{(1)} = -\tau\left[\partial_{t_0}(P(\rho) + \rho u^2) + \partial_x \sum_i \xi_i^3 f_i^{(0)}\right] = -\tau\left[3P - \rho\frac{dP}{d\rho}\right]\frac{\partial u}{\partial x}. \tag{A2}$$

The unusual factor of $3P - \rho\, dP/d\rho$ in the viscosity may be eliminated by making the relaxation time τ a function of the local density, subject always to the constraint $3P - \rho\, dP/d\rho > 0$ so that τ remains positive. This excludes, for example, compressible flow in water. Water behaves like an adiabatic gas ($P \propto \rho^\gamma$) with exponent $\gamma = 7$, for which $3P - \rho\, dP/d\rho = -4P$ is negative.

Preliminary results suggest that there is an $N^{(0)}$ to stabilise the equilibria (A1), but that the dependence on pressure is non-monotonic, unlike the previous choices $N^{(0)} = \frac{1}{2}[\rho - P(\rho)]$ for D1Q5, and $N^{(0)} = \rho - 3P(\rho)$ for D2Q9.

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