# Lecture 3: Generalized Lattice Boltzmann Equation

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# Motivation

- To overcome the shortcomings of the BGK model;
- To improve numerical stability;
- To gain maximan freedom of the model;
- To present a systematic analysis of the LBE method.

# Dissipation, Dispersion, and Galilean Invariance

- Dissipation: Hyperviscosity

$$\nu(\boldsymbol{k}) = \nu_0 - \nu_1 k^2 + \nu_2 k^4 + \cdots + (-1)^n \nu_n k^{2n} + \cdots$$

- Galilean Invariance: In reference frame with velocity $\boldsymbol{V}$

$$\exp[i(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t)] \Longrightarrow \exp[i(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t) - ig(\boldsymbol{k})\boldsymbol{k}\cdot\boldsymbol{V}t]$$

$$g(\boldsymbol{k}) = g_0 - g_1 k^2 + g_2 k^4 + \cdots + (-1)^n g_n k^{2n} + \cdots$$

- Isotropy: Dependence of transport coefficients [$\nu(\boldsymbol{k})$, $\eta(\boldsymbol{k})$, $c_s(\boldsymbol{k})$, and $g(\boldsymbol{k})$] on the direction of $\boldsymbol{k}$

- Analysis: Linear Dispersion Equation & Generalized Hydrodynamics[1,2,3,4,5,6]

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[1] L.-S. Luo, H. Chen, S. Chen, G. Doolen, and Y.-C. Lee, *Phys. Rev. A* **43**:7097 (1991).
[2] P. Grosfils and P. Lallemand, *Europhys. Lett.* **24**:473 (1993).
[3] S.P. Das, H.J. Bussemaker, and M.H. Ernst, *Phys. Rev. E* **48**:245 (1993).
[4] P. Grosfils, J.P. Boon, R. Brito, and M.H. Ernst, *Phys. Rev. E* **48**:2655 (1993).
[5] P. Behrend, R. Harris, and P.B. Warren, *Phys. Rev. E* **50**:4586 (1994).
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# Lattice Boltzmann Equation

Lattice Boltzmann Equation in particle velocity space:

$$f_\alpha(\boldsymbol{x}_i + \boldsymbol{e}_\alpha, t + 1) = f_\alpha(\boldsymbol{x}_i, t) + \Omega_\alpha(f) \tag{1}$$

$$\begin{aligned} \rho(\boldsymbol{x}_i, t) &= \sum_\alpha f_\alpha(\boldsymbol{x}_i, t) \\ \rho\boldsymbol{u}(\boldsymbol{x}_i, t) &= \sum_\alpha \boldsymbol{e}_\alpha f_\alpha(\boldsymbol{x}_i, t) \end{aligned}$$

$$|f(\boldsymbol{x}_i + \boldsymbol{e}_\alpha, t + 1)\rangle = |f(\boldsymbol{x}_i, t)\rangle + |\Omega(f)\rangle \tag{2}$$

# Moment Space

Mapping from the distribution functions $\{f_\alpha | \alpha = 1,\ 2,\ \cdots,\ b\}$ to moments $\{\varrho_\alpha | \alpha = 1,\ 2,\ \cdots,\ b\}$ (for 9-velocity model):

$$
\mathsf{M} \equiv \begin{pmatrix} \langle\rho| \\ \langle e| \\ \langle\varepsilon| \\ \langle j_x| \\ \langle q_x| \\ \langle j_y| \\ \langle q_y| \\ \langle p_{xx}| \\ \langle p_{xy}| \end{pmatrix} \equiv \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{pmatrix}
$$

$$
\equiv \left(|\rho\rangle,\ |e\rangle,\ |\varepsilon\rangle,\ |j_x\rangle,\ |q_x\rangle,\ |j_y\rangle,\ |q_y\rangle,\ |p_{xx}\rangle,\ |p_{xy}\rangle\right)^{\mathsf{T}}
$$

$$
|\varrho\rangle = \mathsf{M}|f\rangle \qquad |f\rangle = \mathsf{M}^{-1}|\varrho\rangle
$$

# Moments

The moments in the 9-velocity model:

| Order | Quantity | |
|---|---|---|
| 0 | Density: | $\rho = \langle \rho \vert f \rangle = \langle f \vert \rho \rangle$ |
| 2 | Energy: | $e = \langle e \vert f \rangle = \langle f \vert e \rangle$ |
| 4 | Energy Square: | $\varepsilon = \langle \varepsilon \vert f \rangle = \langle f \vert \varepsilon \rangle$ |
| 1 | $x$-Momentum: | $j_x = \langle j_x \vert f \rangle = \langle f \vert j_x \rangle$ |
| 3 | $x$-Heat Flux: | $q_x = \langle q_x \vert f \rangle = \langle f \vert q_x \rangle$ |
| 1 | $y$-Momentum: | $j_y = \langle j_y \vert f \rangle = \langle f \vert j_y \rangle$ |
| 3 | $y$-Heat Flux: | $q_y = \langle q_y \vert f \rangle = \langle f \vert q_y \rangle$ |
| 2 | Stress: | $p_{xx} = \langle p_{xx} \vert f \rangle = \langle f \vert p_{xx} \rangle$ |
| 2 | Stress: | $p_{xy} = \langle p_{xy} \vert f \rangle = \langle f \vert p_{xy} \rangle$ |

# Generalized BGK Approximation in Moment Space

Relaxation process of moments:

$$\begin{pmatrix} \Delta\rho \\ \Delta e \\ \Delta\varepsilon \\ \Delta j_x \\ \Delta q_x \\ \Delta j_y \\ \Delta q_y \\ \Delta p_{xx} \\ \Delta p_{xy} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -s_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -s_3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -s_5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -s_7 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -s_8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -s_9 \end{pmatrix} \begin{pmatrix} \delta\rho \\ \delta e \\ \delta\varepsilon \\ \delta j_x \\ \delta q_x \\ \delta j_y \\ \delta q_y \\ \delta p_{xx} \\ \delta p_{xy} \end{pmatrix}$$

$$|\delta\varrho\rangle \equiv |\varrho\rangle - |\varrho^{(\mathrm{eq})}\rangle$$
$$|\Delta\varrho\rangle = \mathsf{S}\left[|\varrho\rangle - |\varrho^{(\mathrm{eq})}\rangle\right]$$

[7] D. d'Humières, in *Rarefied Gas Dynamics: Theory and Simulations*, Prog. Astronaut. Aeronaut. Vol. **159**, edited by B.D. Shizgal and D.P. Weaver (AIAA, Washington, D.C. 1992).

[8] L.-S. Luo and P. Lallemand, *Phys. Rev. E* **61**:6546 (2000).

# Equilibriums in Moment Space

The equilibrium functions depend only upon conserved moments:

$$
\begin{aligned}
e^{(\mathrm{eq})} &= \frac{1}{\langle e|e\rangle}\left[\alpha_2\,\langle\rho|\rho\rangle\,\rho + \gamma_2\,(\langle j_x|j_x\rangle j_x^2 + \langle j_y|j_y\rangle j_y^2)\right] = \frac{1}{4}\alpha_2\,\rho + \frac{1}{6}\gamma_2\,(j_x^2 + j_y^2) \\
\varepsilon^{(\mathrm{eq})} &= \frac{1}{\langle \varepsilon|\varepsilon\rangle}\left[\alpha_3\,\langle\rho|\rho\rangle\,\rho + \gamma_4\,(\langle j_x|j_x\rangle j_x^2 + \langle j_y|j_y\rangle j_y^2)\right] = \frac{1}{4}\alpha_3\,\rho + \frac{1}{6}\gamma_4\,(j_x^2 + j_y^2) \\
q_x^{(\mathrm{eq})} &= \frac{\langle j_x|j_x\rangle}{\langle q_x|q_x\rangle} c_1 j_x = \frac{1}{2} c_1 j_x \\
q_y^{(\mathrm{eq})} &= \frac{\langle j_y|j_y\rangle}{\langle q_y|q_y\rangle} c_1 j_y = \frac{1}{2} c_1 j_y \\
p_{xx}^{(\mathrm{eq})} &= \gamma_1\,\frac{1}{\langle p_{xx}|p_{xx}\rangle}(\langle j_x|j_x\rangle j_x^2 - \langle j_y|j_y\rangle j_y^2) = \frac{3}{2}\gamma_1 (j_x^2 - j_y^2) \\
p_{xy}^{(\mathrm{eq})} &= \gamma_3\,\frac{\sqrt{\langle j_x|j_x\rangle\langle j_y|j_y\rangle}}{\langle p_{xx}|p_{xx}\rangle}(j_x j_y) = \frac{3}{2}\gamma_3 (j_x j_y)
\end{aligned}
$$

There are 7 adjustable parameters in the model: $\alpha_2$, $\alpha_3$, $c_1$, $\gamma_1$, $\gamma_2$, $\gamma_3$, $\gamma_4$.

# Generalized Lattice Boltzmann Equation

Generalized Lattice Boltzmann Equation with multiple relaxation parameters:

$$|f(\boldsymbol{x}_i + \boldsymbol{e}_\alpha,\, t+1)\rangle = |f(\boldsymbol{x}_i,\, t)\rangle + \mathsf{M}^{-1}\mathsf{S}\left[|\varrho(\boldsymbol{x}_i,\, t)\rangle - |\varrho^{(\mathrm{eq})}(\boldsymbol{x}_i,\, t)\rangle\right] \tag{3}$$

- Initialize $|f\rangle$;
- Project $|f\rangle$ to moments by $|\varrho\rangle = \mathsf{M}|f\rangle$ and compute the equilibrium $|\varrho^{(\mathrm{eq})}\rangle$;
- Collision in moment space (multiple-parameter relaxation)

$$|\Delta\varrho\rangle \equiv \mathsf{S}\left[|\varrho\rangle - |\varrho^{(\mathrm{eq})}\rangle\right]$$

- Streaming in velocity space:

$$|f(\boldsymbol{x}_i + \boldsymbol{e}_\alpha,\, t+1)\rangle = |f(\boldsymbol{x}_i,\, t)\rangle + \mathsf{M}^{-1}|\Delta\varrho\rangle$$

# Linearized Lattice Boltzmann Equation

Suppose the system in uniform state $\rho$ and $\boldsymbol{V} = (V_x,\, V_y)$, and

$$|f\rangle = |f^{(0)}\rangle + |\delta f\rangle$$

$$|\delta f(\boldsymbol{r}_j + \boldsymbol{e}_\alpha,\, t+1)\rangle = |\delta f(\boldsymbol{r}_j,\, t)\rangle + \mathsf{M}^{-1}\mathsf{C}\mathsf{M}|\delta f(\boldsymbol{r}_j,\, t)\rangle$$

In Fourier space:

$$\mathsf{A}|\delta f(\boldsymbol{k},\, t+1)\rangle = |\delta f(\boldsymbol{k},\, t)\rangle + \mathsf{M}^{-1}\mathsf{C}\mathsf{M}|\delta f(\boldsymbol{k},\, t)\rangle$$

$$\mathsf{C}_{\alpha\beta} = \frac{\langle \varrho_\alpha | \varrho_\alpha \rangle}{\langle \varrho_\beta | \varrho_\beta \rangle} \frac{\partial}{\partial \varrho_\alpha} [\varrho_\beta - \varrho_\beta^{(\mathrm{eq})}] \qquad \mathsf{A}_{\alpha\beta} = \exp(i\boldsymbol{e}_\alpha \cdot \boldsymbol{k})\, \delta_{\alpha\beta}$$

The Linearized Lattice Boltzmann Equation:

$$|\delta f(\boldsymbol{k},\, t+1)\rangle = \mathsf{L}|\delta f(\boldsymbol{k},\, t)\rangle \qquad \mathsf{L} = \mathsf{A}^{-1}[\mathsf{I} + \mathsf{M}^{-1}\mathsf{C}\mathsf{M}] \tag{4}$$

# Eigenvalue Problem of Linearized LBE

The eigenvalue problem of the linearized evolution operator:

$$\det[\mathsf{L} - z\mathsf{I}] = 0$$

Hydrodynamic modes ($z_\alpha = 1$) of $\mathsf{L}$ at $\boldsymbol{k} = (k\cos\theta,\, k\sin\theta) \to \boldsymbol{0}$:

$$|\varrho_T\rangle = \cos\theta|j_x\rangle - \sin\theta|j_y\rangle \equiv |j_T\rangle$$
$$|\varrho_\pm\rangle = |\rho\rangle \pm (\cos\theta|j_x\rangle + \sin\theta|j_y\rangle) \equiv |\rho\rangle \pm |j_L\rangle$$

$$|\varrho_T(t)\rangle = {z_T}^t\,|\varrho_T(0)\rangle = \exp[-ik(gV\cos\phi)t]\exp(-\nu k^2 t)|\varrho_T(0)\rangle$$
$$|\varrho_\pm(t)\rangle = {z_\pm}^t\,|\varrho_\pm(0)\rangle = \exp[\pm ik(c_s \pm gV\cos\phi)t]\exp[-(\nu/2+\zeta)k^2 t]|\varrho_\pm(0)\rangle$$

Transport coefficients $\nu$, $\zeta$, $c_s$, and $g$ are functions of wavevector $\boldsymbol{k}$.

# Determining Adjustable Parameters

Galilean invariance of the phases in the transverse mode ($z_T$) and the sound modes ($z_\pm$) up to $\boldsymbol{k}$ leads to:

$$\gamma_1 = \gamma_3 = \frac{2}{3}$$
$$\gamma_2 = 18$$

Isotropy of the attenuation of the transverse mode ($z_T$) and Galilean invariance of the attenuation of the sound modes ($z_\pm$) lead to

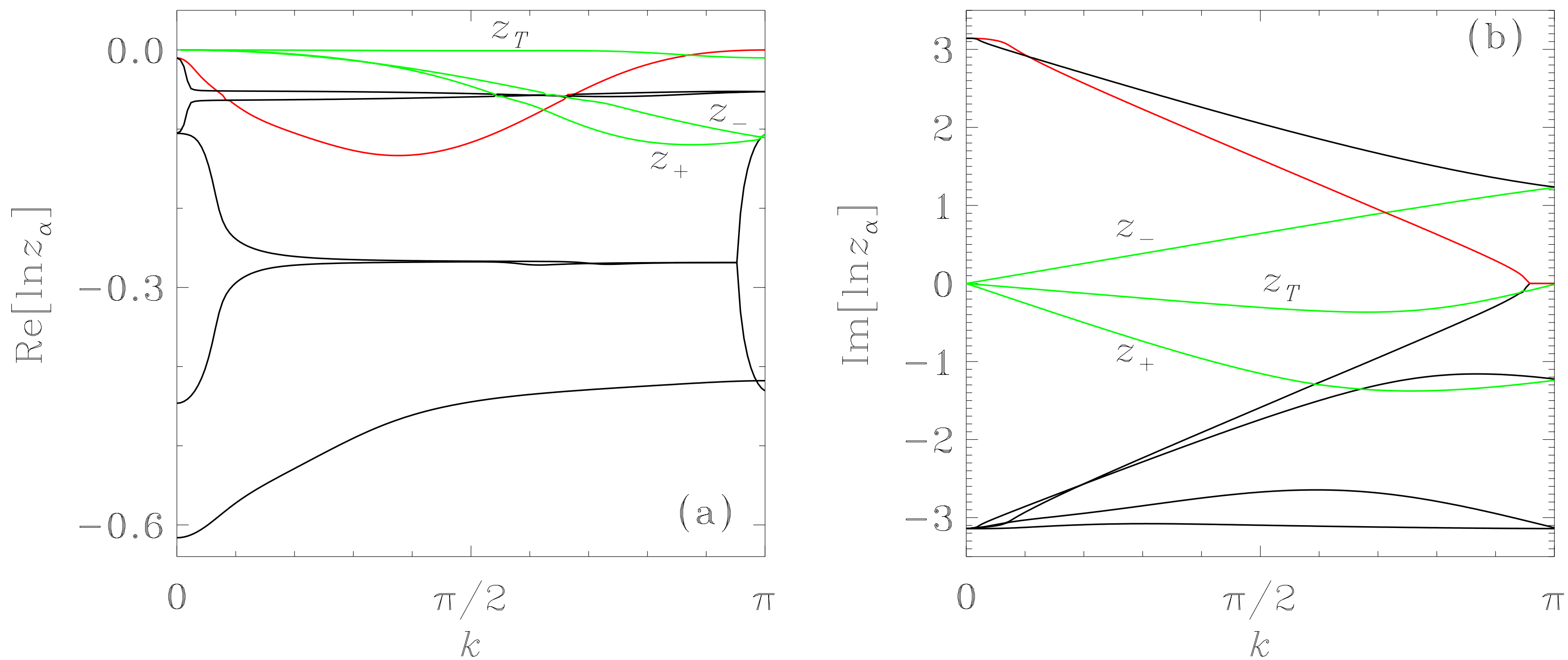
$$c_1 = -2 \qquad (c_s = 1/\sqrt{3})$$
$$\alpha_2 = -8$$

Remaining adjustable parameters: $\alpha_3$ and $\gamma_4$ (in $\epsilon^{(\mathrm{eq})}$). If

$$\alpha_3 = 4 \qquad \gamma_4 = -18 \qquad s_\alpha = \frac{1}{\tau}$$

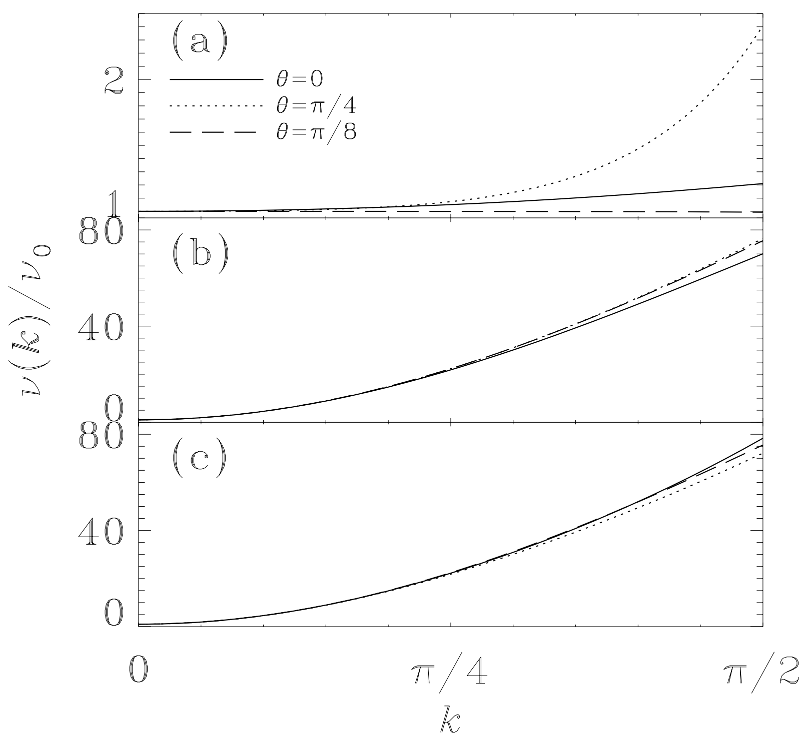
Generalized lattice Boltzmann equation degenerates to a lattice BGK model.

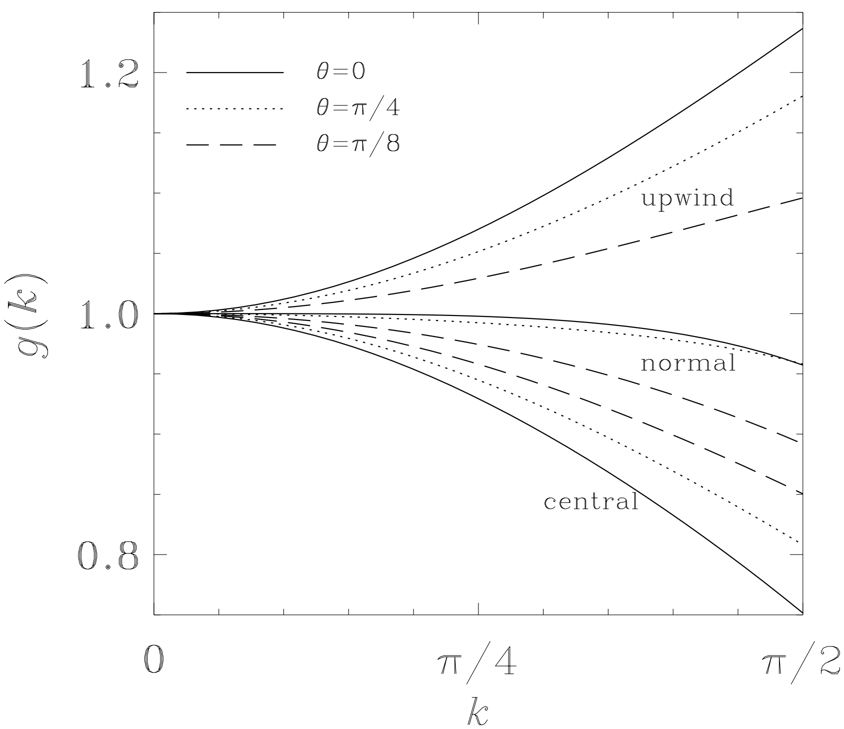
# Behaviors of Eigenvalues of L




Logarithmic eigenvalues of the nine-velocity model. The values of the parameters are $\alpha_2 = -8$, $\alpha_3 = 4$, $c_1 = -2$, $\gamma_1 = \gamma_3 = 2/3$, $\gamma_2 = 18$, and $\gamma_4 = -18$. The relaxation parameters are: $s_2 = 1.64$, $s_3 = 1.54$, $s_5 = s_7 = 1.9$, and $s_8 = s_9 = 1.99$. The streaming velocity $\boldsymbol{V}$ is parallel to $\boldsymbol{k}$ with $V = 0.2$, and $\boldsymbol{k}$ is along the $x$ axis. (a) $\mathrm{Re}(\ln z_\alpha)$ and (b) $\mathrm{Im}(\ln z_\alpha)$.

# Behaviors of Transport Coefficients

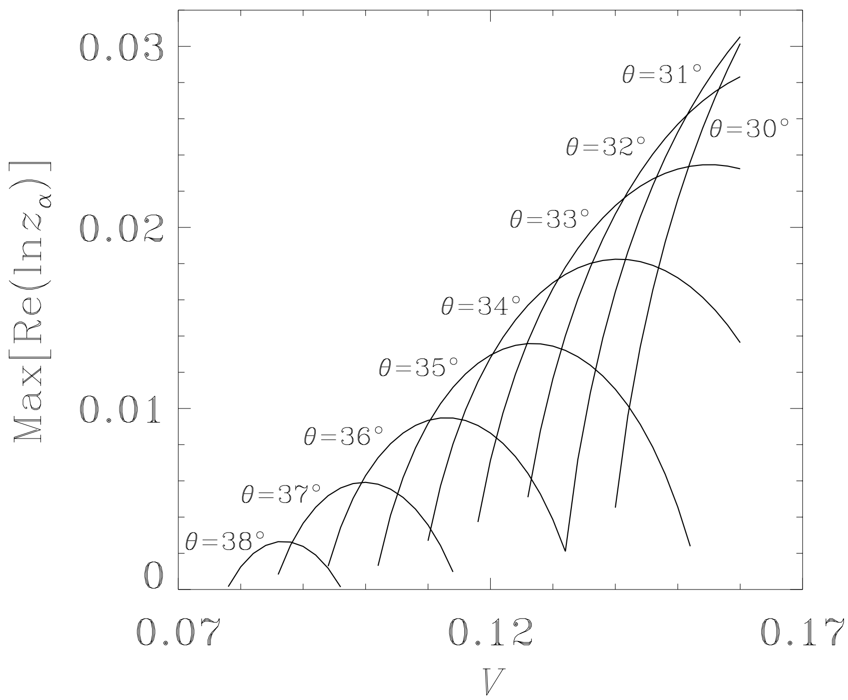


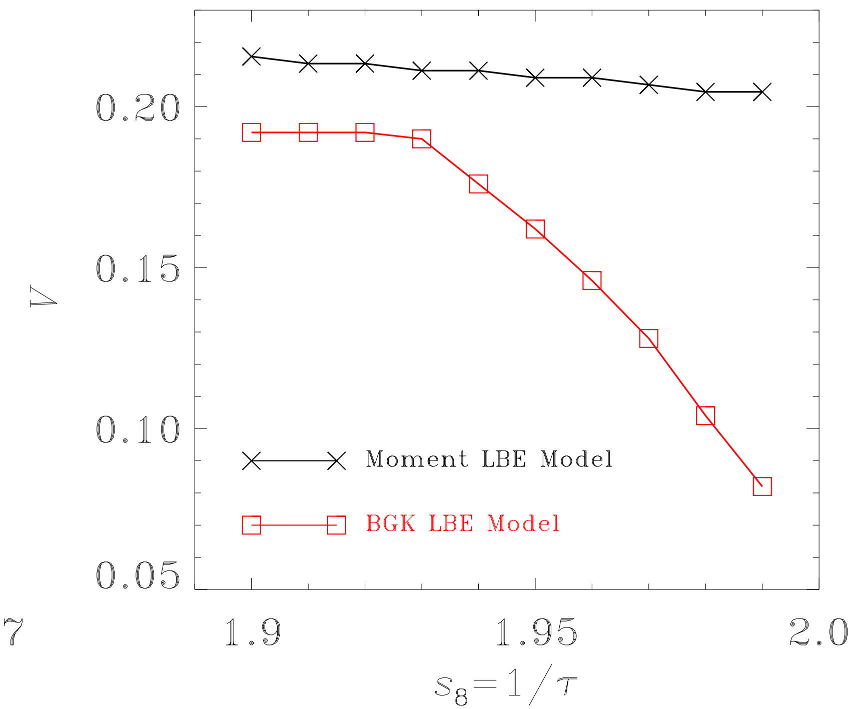




$\boldsymbol{k}$ dependence of viscosities and $g$-factor. The solid lines, dotted lines, and dashed lines correspond to $\theta = 0$, $\pi/8$, and $\pi/4$, respectively. LBE model (1) with no interpolation, (2) with central interpolation, and (3) with upwind interpolation.

# Local Stability Analysis

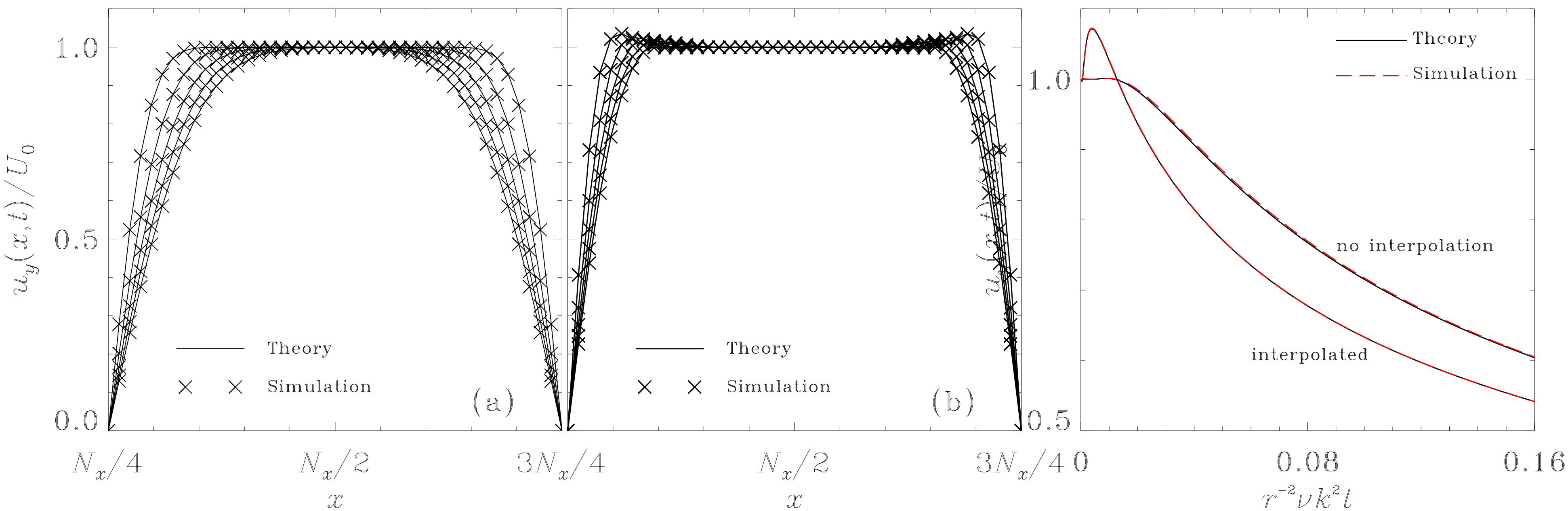
If $\mathrm{Re}(\ln z_\alpha) > 0$, mode $|\varrho_\alpha\rangle$ is unstable.



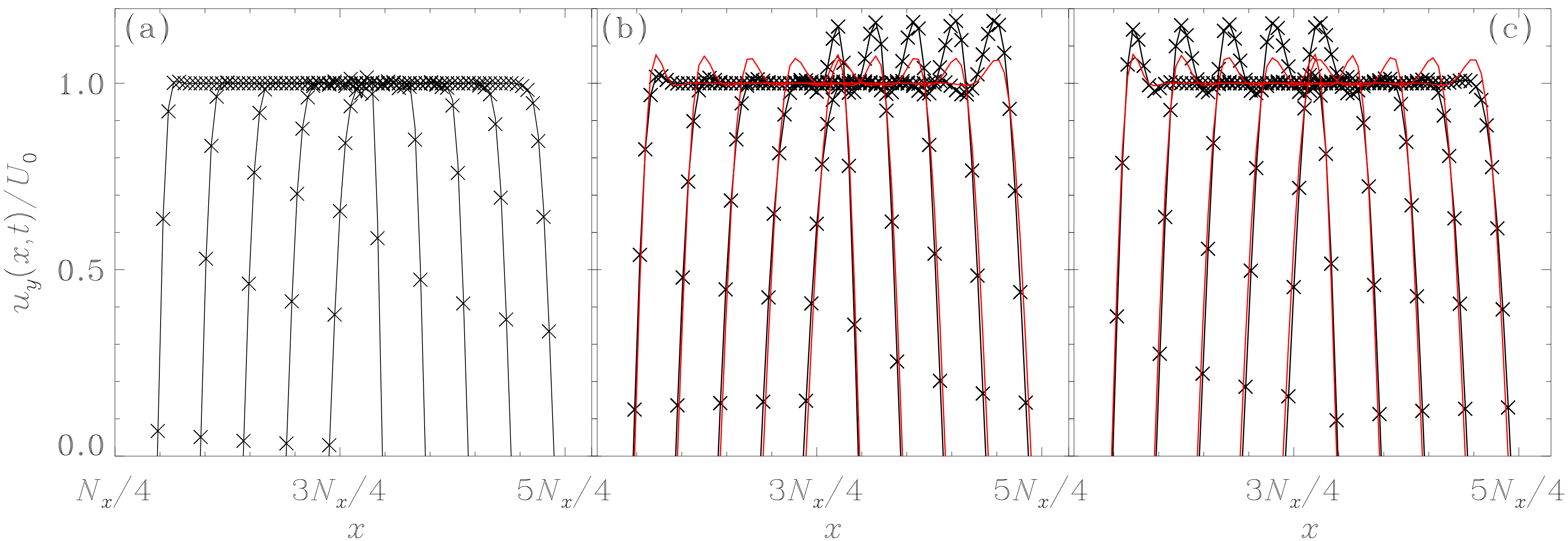

Stability of the generalized LBE model *vs.* the BGK LBE model in the parameter space of $V$ and $s_8 = 1/\tau$. (left) $\max[\mathrm{Re}(\ln z_\alpha)]$ for given $\boldsymbol{V}$. (right) Stability region of GLBE *vs.* LBGK model.

# Artifacts of the LBE Method




Decay of discontinuous shear wave velocity profile $u_y(x, t)$. The lines and symbols ($\times$) are theoretical and numerical results, respectively. Only the positive half of each velocity profile is shown. LBE model (a) with no interpolation, (b) with the central interpolation and $r = 0.5$. (right) at a location close to the discontinuity $x = 3N_x/4$. The time is rescaled as $r^{-2}\nu k^2 t$.

# Artifacts of the LBE Method




Decay of discontinuous shear wave velocity profile $u_y(x, t)$ with a constant streaming velocity $V_x = 0.08 = U_0$. The solid lines and symbols (×) are theoretical and numerical results, respectively. The dashed lines in (b) and (c) are obtained by setting $g_n = 1$. (a) no interpolation, (b) central interpolation and $r = 0.5$, (c) upwind interpolation and $r = 0.5$.

# Conclusions

- The Generalized LBE is superior than the Lattice BGK model;
- Analysis of the (linear) dispersion equation is equivalent to the Chapman-Enskog analysis, while Chapman-Enskog analysis is not valid for situation of finite wavevector $\boldsymbol{k}$;
- Analysis of the (linear) dispersion equation is also applicable to complex fluids (*e.g.*, viscoelastic fluids).
- Limitations of the dispersion equation analysis:
  - Nonlocal effects (gradients);
  - Boundary conditions.