清華大學
Tsinghua University

Hydrodynamic transport at micro- and nanoscales: from molecules to phonons and electrons

Yunfan Huang
Department of Engineering Mechanics
Tsinghua University
2024.06.13

Multiscale Interfacial Transport Laboratory

Contents

- Introduction to viscous fluid mechanics
- Hydrodynamics in quantum transport
  - From molecules to electrons and phonons
- Physics in multiscale models
  - Mesoscopic results: Novel phenomena and DOM method
  - Macroscopic description: Up-scaling and N-S equations
- Conclusions

Contents

- Introduction to viscous fluid mechanics
- Hydrodynamics in quantum transport
  - From molecules to electrons and phonons
- Physics in multiscale models
  - Mesoscopic results: Novel phenomena and DOM method
  - Macroscopic description: Up-scaling and N-S equations
- Conclusions

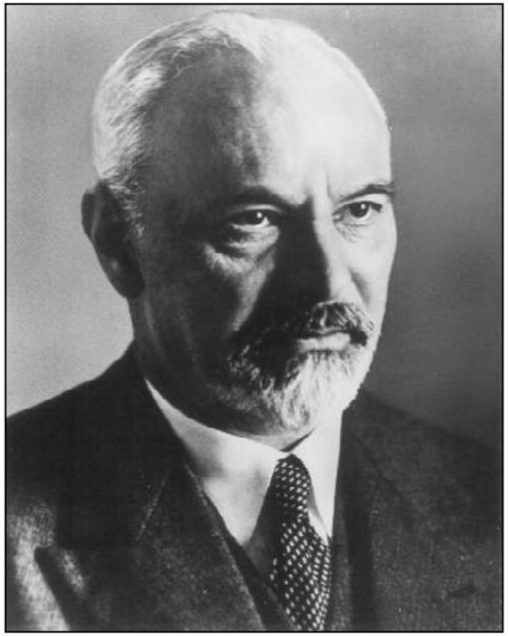
A first view …

洋流与梵高的画

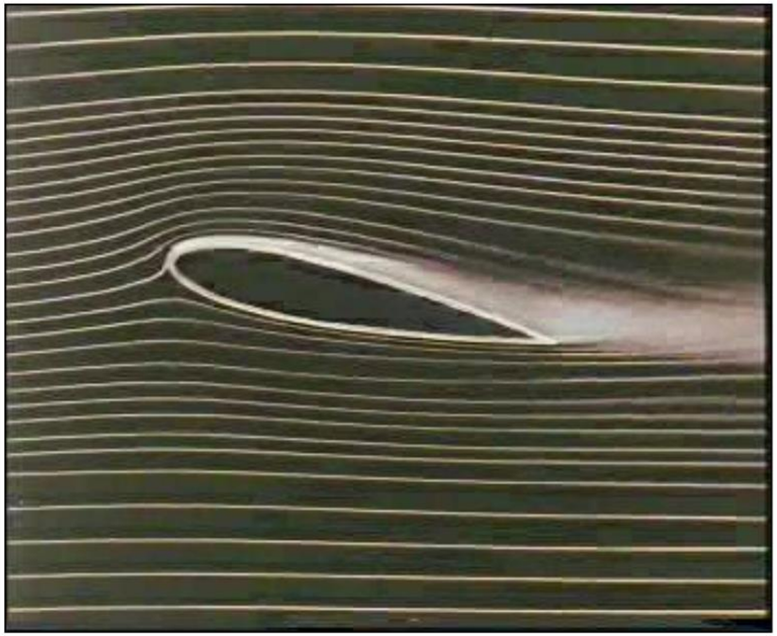
[1] Refer to 粘性流体力学 (黄伟希老师)

L. Prandtl: boundary layer theory

二十世纪三位最杰出的流体力学大师和主要贡献



L. Prandtl (1875-1953)



边界层理论（动画1, 2）

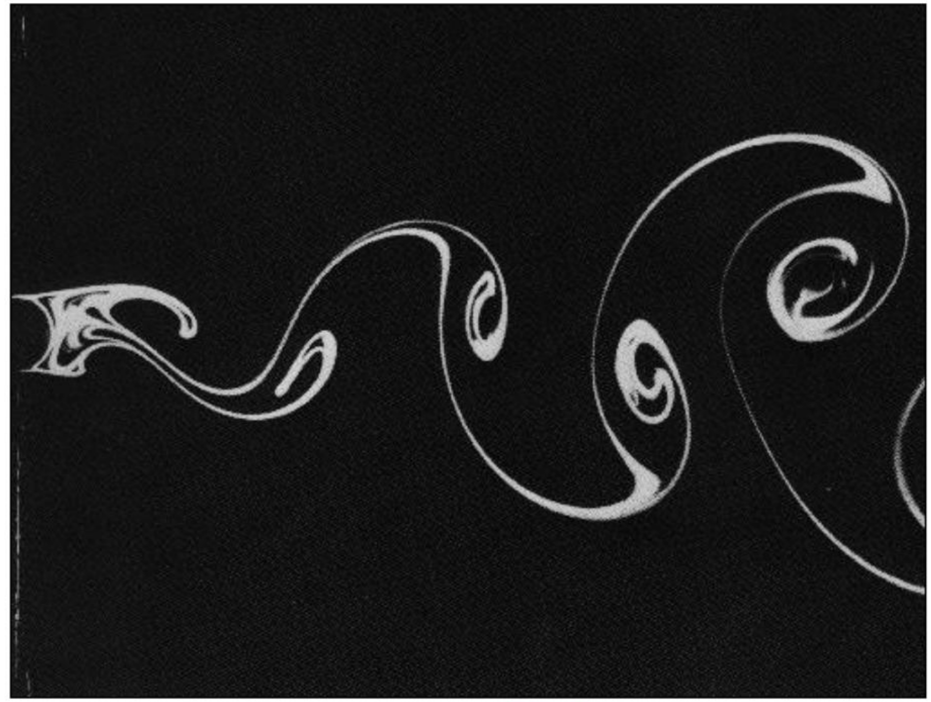
Ludwig Prandtl and his Kaiser-Wilhelm-Institute, *Annual Review of Fluid Mechanics*, 1987, Vol. 19

朱克勤，普朗特和他的流体力学研究所，力学与实践, 2015, 37(3): 400-404

[1] Refer to 粘性流体力学 (黄伟希老师)

T. von Karman: Karman vortex street

T. von Kárman
(1881-1963)



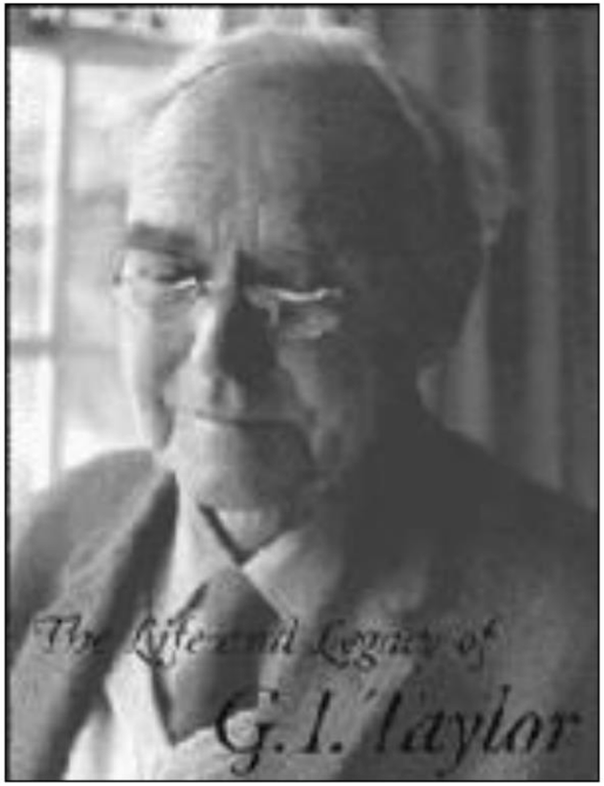
Kárman涡街

The Karman Years at GALCIT, *Annual Review of Fluid Mechanics*, 1979, 11

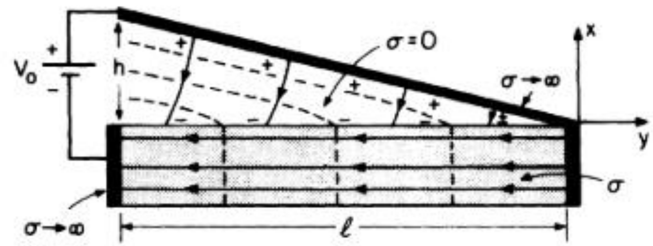
朱克勤，二十世纪的力学大师冯卡门，力学与实践, 2003, 25(2):74-75

[1] Refer to 粘性流体力学 (黄伟希老师)

G. I. Taylor: Taylor pump & Taylor vortex



G.I.Taylor (1886-1975)



Taylor 电流体泵

Taylor 涡（动画1， 2）

G. I. Taylor in His Later Years, *Annual Review of Fluid Mechanics*, 1997, 29

[1] Refer to 粘性流体力学 (黄伟希老师)

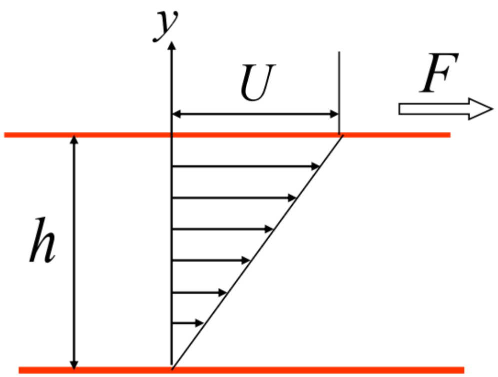
Viscosity, Newton's law, and NS equations

粘性是流体运动时所呈现出的抵抗剪切变形的一种物理属性

粘性是指施加于流体的应力和由此产生的变形速率以一定的关系联系起来的流体的一种宏观属性。

<u>牛顿内摩擦定律</u>

$$\tau = \mu \frac{U}{h}$$



$$u = \frac{U}{h} y$$

$$\tau = \mu \frac{\mathrm{d}u}{\mathrm{d}y}$$

动力粘性系数 μ $[\mathrm{Pa \cdot s}]$ （动画）

$$\partial_t \tilde{\boldsymbol{u}} + (\tilde{\boldsymbol{u}} \cdot \nabla)\tilde{\boldsymbol{u}} = -\nabla \tilde{p} + \nu \Delta \tilde{\boldsymbol{u}} + \nabla \cdot \tilde{\boldsymbol{\tau}}, \quad \nabla \cdot \tilde{\boldsymbol{u}} = 0$$

$$Re = \rho U L / \mu$$

[1] Refer to 粘性流体力学 (黄伟希老师)

Microscopic mechanism of viscosity

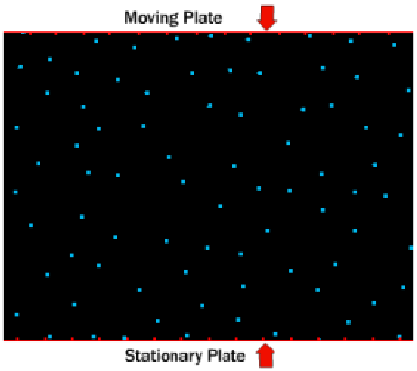
流体是分子组成的，任何宏观现象本质上是由微观分子特性及运动所确定

液体分子间的相互作用力是产生粘性的重要原因之一。对于气体，分子间的相互作用用非常弱，粘性源于分子热运动导致的动量输运。

分子输运	质量	动量	热量
宏观效应	质量扩散	粘性	热传导

产生以上效应的基本原因：

1. 分子不规则热运动；
2. 密度场、速度场和温度场存在空间梯度，处于非平衡状态

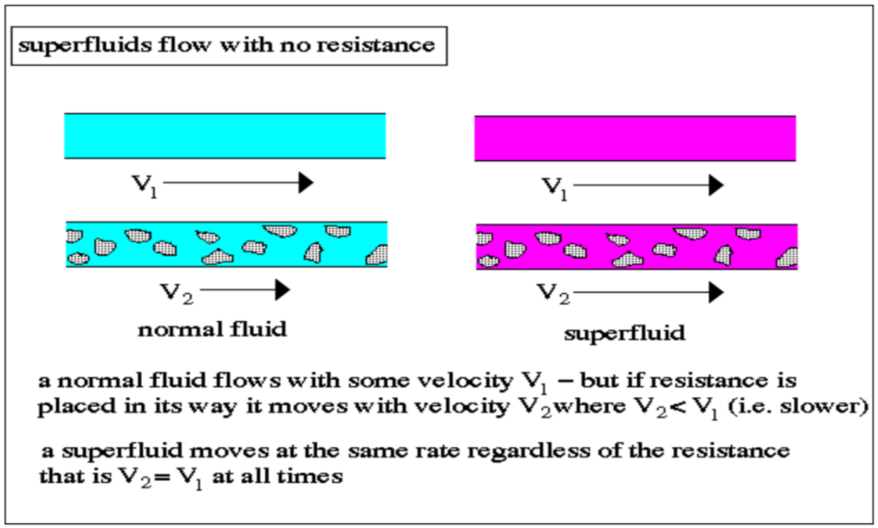


思考：温度上升，气体和液体的粘性怎么变化？

[1] Refer to 粘性流体力学 (黄伟希老师)

What if viscosity disappears?

$He^4 - I$（正常流体相）　$He^4 - II$（超流相）



超流现象涉及量子效应，作为低温物理的两大支柱之一，有关超流的研究在1962、1978、1996 和2003已先后四次获诺贝尔物理奖。值得关注，但需要坚实的理论物理和流体力学基础。

Henderson, K. L. & Barenghi, C. F. Transition from Ekman flow to Taylor vortex flow in superfluid helium, *Journal of Fluid Mechanics* 2004, 508, 319–331.

Henderson, K. L. & Barenghi, C. F. The anomalous motion of superfluid helium in a rotating cavity. *J. Fluid Mech*. 2000 , 406, 199–219.

Statistical Hydrodynamics. (*)

L. Onsager

New Haven, Conn.

It is a familiar fact of hydrodynamics, than when the « Reynolds number » exceeds a certain critical value, which depends on the type of flow, no steady flow is stable. The unsteady flow which occurs under these conditions calls for statistical analysis; but early attempts in this direction encountered formidable difficulties. Within the last few years, however, the most important remaining questions concerning the stability of laminar flow were settled by C. C. Lin [1], and a promising start towards a quantitative theory of turbulence was achieved by Kolmogoroff [2]. For good measure, Kolmogoroff's main result was rediscovered at least twice [3], [4]. The theories involved deal with the mechanism of turbulent dissipation. We shall return to this subject; it seems logical to discuss first a different, new application of statistics to hydrodynamics.

It is of some interest to note that in principle, turbulent dissipation as described could take place just as readily **without the final assistance by viscosity**. In the absence of viscosity, the standard proof of the conservation of energy does not apply, because the velocity field does not remain differentiable! In fact it is possible to show that the velocity field in such 'ideal' turbulence cannot obey any LIPSCHITZ condition of the form

$$|\boldsymbol{v}(\boldsymbol{r}' + \boldsymbol{r}) - \boldsymbol{v}(\boldsymbol{r}')| < (\text{const.})r^n$$

Superfluid (Onsager)

Ideal turbulence (Onsager)

[1] Andronikashvili, E.L. and Y.G. Mamaladze, Quantization of Macroscopic Motions and Hydrodynamics of Rotating Helium II. *Reviews of Modern Physics*, 1966. **38**(4): 567-625.
[2] Onsager, L., Statistical hydrodynamics. Il Nuovo Cimento (1943-1954), 1949, **6**(Suppl 2): 279-287.

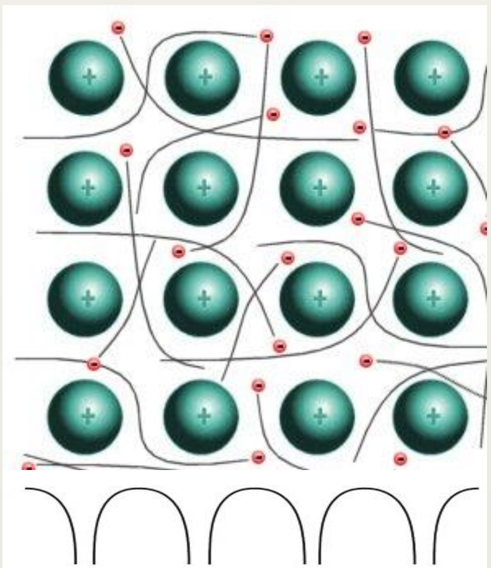
Contents

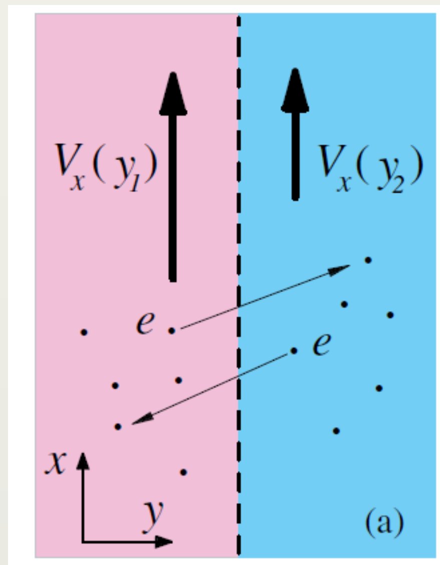
- Introduction to viscous fluid mechanics
- Hydrodynamics in quantum transport
  - From molecules to electrons and phonons
- Physics in multiscale models
  - Mesoscopic results: Novel phenomena and DOM method
  - Macroscopic description: Up-scaling and N-S equations
- Conclusions

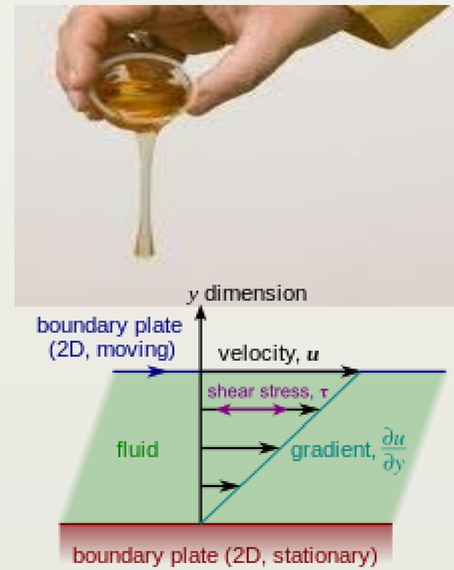
Viscosity emerges from the electron transport

Room/ultralow temperature ⟶ Low temperature & low dimension & ultrapure

- Metal, Si|Ga[Al]As, Doped-S|BLG, Pt|PdCoO$_2$
- SLG, semi-metal (MoP, WP$_2$), topo-insulator







Nearly Free electron model	Viscous electron model	Viscous fluid model
Electron⟷ Lattice*	Electron⟷Electron** ⟷	Molecular⟷Molecular

Lattice-induced resistance

(Ohmic flow)

Boundary-induced resistance

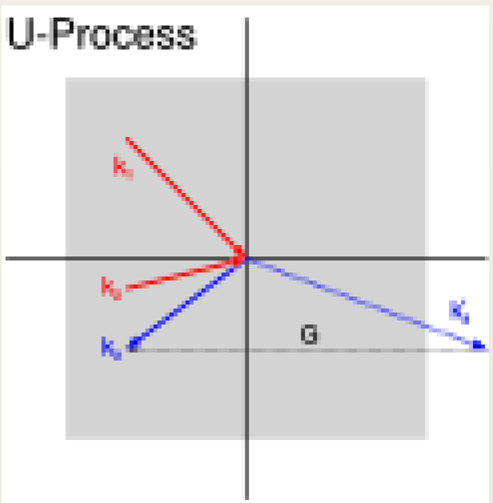
(Hydrodynamic flow)

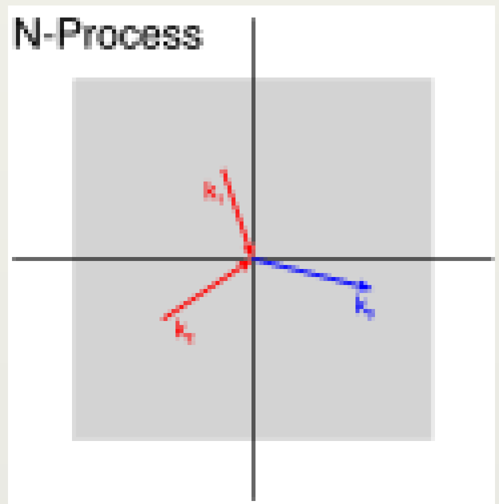
* Refers to phonons and defects.
** Direct scattering or mediated by phonons

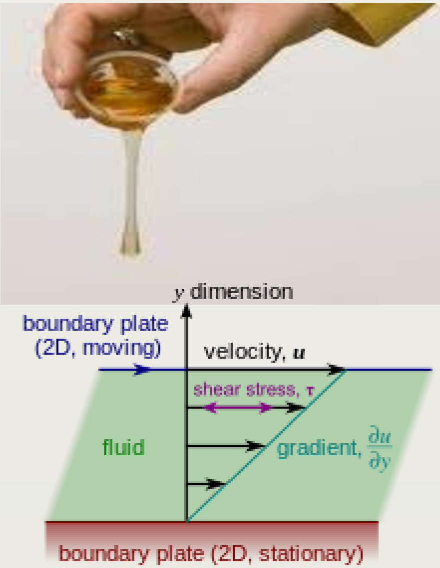
Electron hydrodynamics!

What about phonons?

Room temperature ⟶ Low temperature







Classical model	Hydrodynamic model	Viscous fluid model
Phonon ⟷ Phonon (U)	$\boxed{\text{Phonon} \leftrightarrow \text{Phonon (N)}}$ ⟷	Molecular ⟷ Molecular

Umklapp-induced resistance
(Fourier law)

Boundary-induced resistance
(Hydrodynamic flow)

Phonon hydrodynamics!

Hydrodynamic transport: Parallel treatment

- **Boltzmann transport equation (BTE) – semi-classical description**

collective moving velocity

$$\boxed{\frac{\mathrm{d}f}{\mathrm{d}t}} = \frac{\partial f}{\partial t} + \boldsymbol{v}\cdot\frac{\partial f}{\partial \boldsymbol{r}} + \frac{\boldsymbol{F}}{m}\cdot\frac{\partial f}{\partial \boldsymbol{v}} = \boxed{C(f)} \begin{cases} \text{Resistive scattering} & f_0(\boldsymbol{r}, \varepsilon_k) \\ \text{Conservative scattering} & f_0(\boldsymbol{r}, \varepsilon_k - \boldsymbol{u}\cdot\boldsymbol{p}) \end{cases}$$

Change of particle state ⟸ **Particle scattering** **Different mechanisms** ⟹ **Different (quasi-) equilibrium states**

f: the non-equilibrium distribution function of the particle cluster around $(\boldsymbol{r}, \boldsymbol{v})$

Solving BTE: Deterministic | Stochastic (particle nature)

Upscaling BTE: Hydrodynamic description (macroscopic)

Beyond BTE: *wave nature, strong correlation, scattering rate*

<u>*Coherence*</u>: *Quantum transport in low-D system*

<u>*Localization*</u>: *Strong disordered/correlated system*

<u>*Super/Magneto/Topo*</u>: *Strong (spin/Coulomb) correlated system*

Chen G. *Nanoscale Energy Transport and Conversion*. Tsinghua University Press. 2014

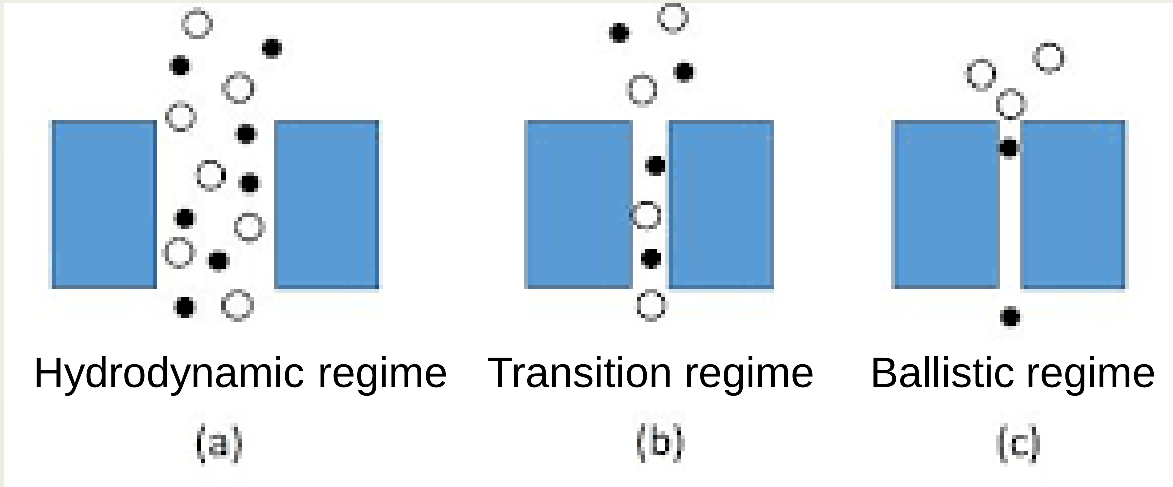
Contents

- Introduction to viscous fluid mechanics
- Hydrodynamics in quantum transport
  - From molecules to electrons and phonons
- Physics in multiscale models
  - Mesoscopic results: Novel phenomena and DOM method
  - Macroscopic description: Up-scaling and N-S equations
- Conclusions

Knudsen effect in gas transport at microscale

$v \sim \overline{u}\, l_{\mathrm{mm}}$

$l_{\mathrm{eff}} \sim d^2 / l_{\mathrm{mm}}$



$l_{\mathrm{eff}} \sim W$

MINIMUM OF RESISTANCE IN IMPURITY-FREE CONDUCTORS

R. N. GURZHI

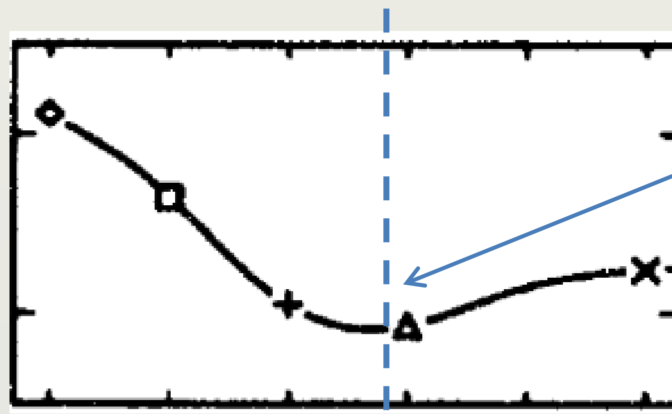
Submitted to JETP editor December 21, 1962

J. Exptl. Theoret. Phys. (U.S.S.R.) 44, 771-772 (February, 1963)

the first paper on
electron hydrodynamics

$\sigma = Q/\Delta p$

$\sim l_{\mathrm{eff}}$



Knudsen minimum

collective continuum flow

0.001

$\mathrm{Kn} = \dfrac{l_{\mathrm{mm}}}{W}$

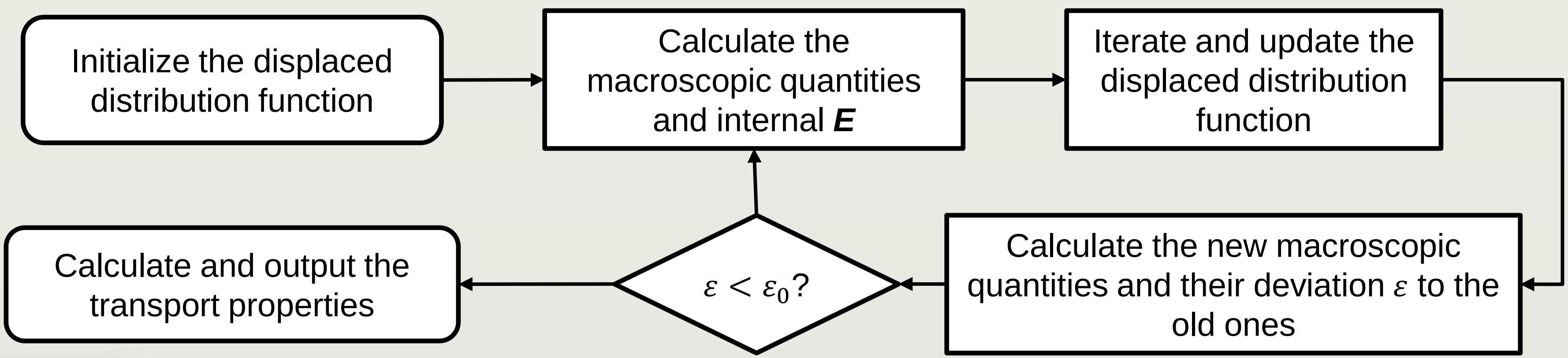
100

“**Free** molecular” flow

[1] Gurzhi R N. *Sov. Phys. JETP.*, 1963, **17**: 521.
[2] De Jong M.J.M, Molenkamp W. *Phys. Rev. B*, 1995, **51**: 13389-13402.

DOM to solve the Boltzmann transport equation

- Discrete Ordinate Method **(DOM)**
  - **Used** to solve phonon BTE in history
  - **Simple** and **clear** for directly discretizing the BTE (upwind scheme)
  - **Appropriate** to simple geometry (mechanism research)
  - **Similar** to Lattice Boltzmann Method
- Protocols of DOM

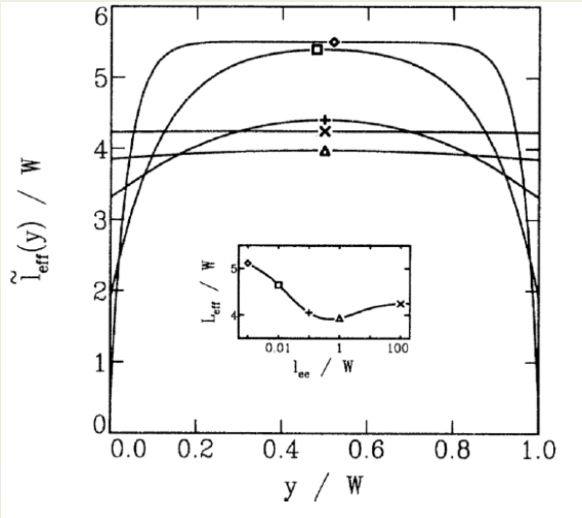


[1] De Jong M.J.M, Molenkamp W. *Phys. Rev. B*, 1995, **51**: 13389-13402.
[2] Huang, Y. and M. Wang. *Physical Review B*, 2021. **104**(15): 155408.

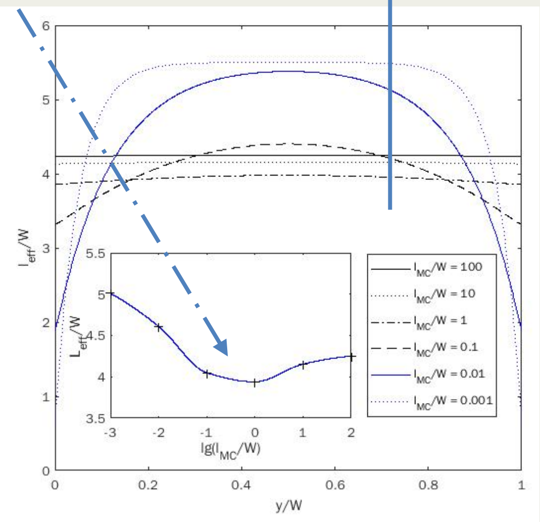
Knudsen-Gurzhi effect in electrons and phonons

Knudsen-Gurzhi **minimum**

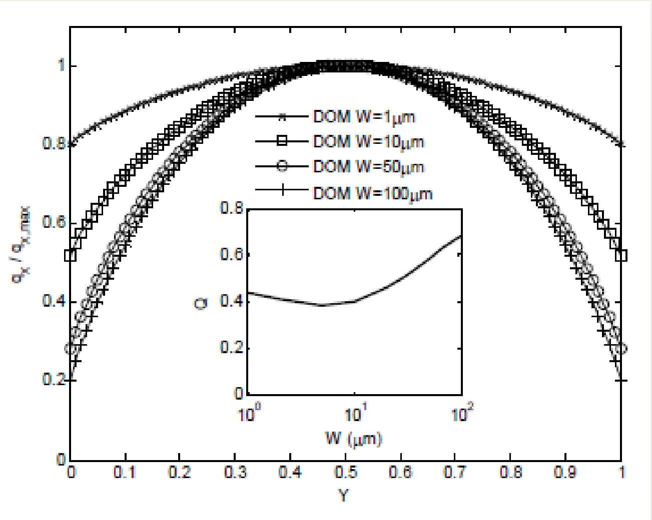
As l_{ee} decreases, **parabolic flow** recovers



Theoretical results (eBTE)



DOM results of (eBTE)



DOM results of (phBTE)

Main figure: velocity profile

Subfigure: conductivity

- **Knudsen**: size effect of gas transport
- **Gurzhi**: electron hydrodynamics

[1] De Jong M.J.M, Molenkamp W. *Phys. Rev. B*, 1995, **51**: 13389-13402.
[2] Huang, Y. and M. Wang. *Physical Review B*, 2021. **104**(15): 155408.
[3] Guo Y (郭洋裕). *Doctor Dissertation*. Tsinghua University, 2018.

Contents

- Introduction to viscous fluid mechanics
- Hydrodynamics in quantum transport
  - From molecules to electrons and phonons
- Physics in multiscale models
  - Mesoscopic results: Novel phenomena and DOM method
  - Macroscopic description: Up-scaling and N-S equations
- Conclusions

Hydrodynamic transport: Characteristics

<table>
<tr><th>Particle</th><th colspan="2">Scattering</th><th>Resistance</th><th>Equations</th></tr>
<tr><td>Molecules</td><td>m-m</td><td rowspan="3">(quasi-) momentum is conservative</td><td rowspan="3">boundary-induced</td><td>N-S equations</td></tr>
<tr><td>Phonons</td><td>ph-ph (N)</td><td>?</td></tr>
<tr><td>Electrons</td><td>e-e (N)</td><td>?</td></tr>
</table>

- Characteristics
  - ✓ "Non-local": collective motion rather than individuals (conservative quantity)
  - ✓ Emergent Phenomena: bulk viscosity emerges from the conservative scattering
  - ✓ Source of resistance: boundary scattering makes the major resistance
- Requirements for phonons and electrons
  - ✓ **Quasi-classical regime**: particle view holds under certain circumstance
  - ✓ **Low temperature and pure**: momentum-conserving scattering dominates
  - ✓ **Micro/nanoscale (low-dim)**: boundary/impurity/dislocation plays essential roles

Chen G. *Nanoscale Energy Transport and Conversion*. Tsinghua University Press. 2014

Upscaling of Boltzmann transport equation

- **Boltzmann transport equation (BTE) – Chapman-Enskog expansion**

$$\frac{\mathrm{d}f}{\mathrm{d}t}=\frac{\partial f}{\partial t}+\boldsymbol{v}\cdot\frac{\partial f}{\partial \boldsymbol{r}}+\frac{\boldsymbol{F}}{m}\cdot\frac{\partial f}{\partial \boldsymbol{v}}=C(f) \qquad f=f^{(0)}+\epsilon f^{(1)}+\epsilon^2 f^{(2)}+\ldots$$

- **Classical N-S equation**

$$\frac{\mathrm{D}\boldsymbol{P}}{\mathrm{D}t}+\nabla\cdot\boldsymbol{\sigma}=\rho\boldsymbol{g} \qquad \boldsymbol{\sigma}=p\boldsymbol{I}-\mu\left(\frac{2}{3}(\nabla\cdot\boldsymbol{u})\boldsymbol{I}+\nabla\boldsymbol{u}+(\nabla\boldsymbol{u})^T\right)$$

- **Phonon N-S equation**

$$\boxed{\frac{\partial \boldsymbol{q}}{\partial t}}+\nabla\cdot\boldsymbol{Q}=-\frac{\boldsymbol{q}}{\tau_{\mathrm{R}}} \qquad \boldsymbol{Q}=\frac{1}{3}v_{\mathrm{g}}^2 e\boldsymbol{I}-\frac{1}{5}v_{\mathrm{g}}^2\tau_{\mathrm{N}}\left((\nabla\cdot\boldsymbol{q})\boldsymbol{I}+\nabla\boldsymbol{q}+(\nabla\boldsymbol{q})^T\right)$$

- **Electron N-S equation**

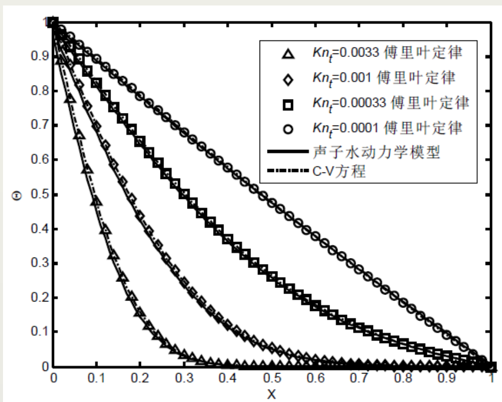
$$\frac{\partial \boldsymbol{P}}{\partial t}+\boxed{\nabla\cdot\boldsymbol{T}}=-\frac{\boldsymbol{P}}{\tau_{\mathrm{MR}}}+m^*\boldsymbol{F}_{\mathrm{macro}} \qquad \boldsymbol{T}=\mathcal{P}\boldsymbol{I}-\mu_{\mathrm{e}}\left((\nabla\cdot\boldsymbol{u})\boldsymbol{I}+\nabla\boldsymbol{u}+(\nabla\boldsymbol{u})^T\right)$$

[1] Guo Y (郭洋裕). *Doctor Dissertation*. Tsinghua University, 2018.
[2] Huang Y (黄云帆). *Undergraduate Thesis*. Tsinghua University, 2019.

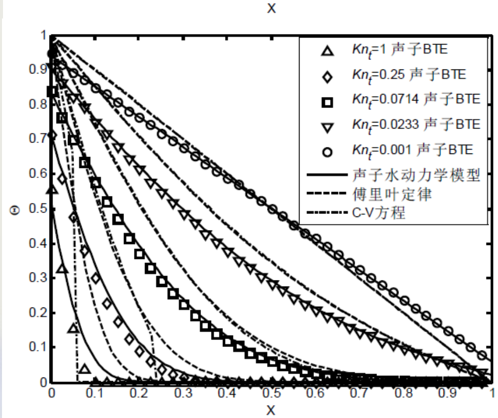
Applications of general Navier-Stokes equations

Transient phonon transport normal to the thin film

$Kn_x = 0.01$



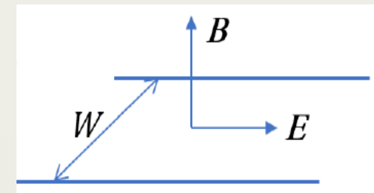
$Kn_x = 0.1$



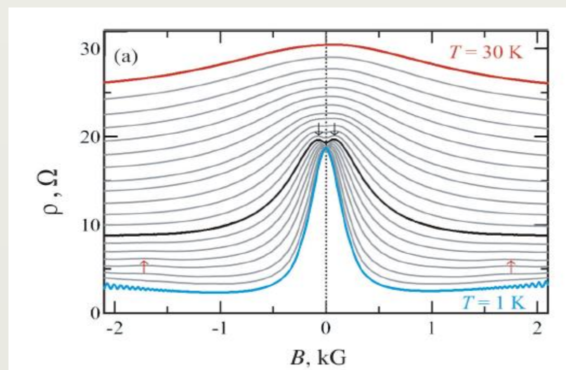
Magneto-hydrodynamic transport of electron

$$\nu_\omega = \frac{v_F^2}{4}\frac{{\tau_{\text{eff}}}^{-1} - i\omega}{({\tau_{\text{eff}}}^{-1} - i\omega)^2 + 4\omega_C^2}$$

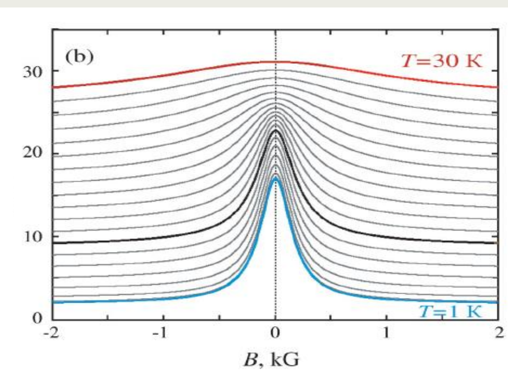
$$\nu_{H,\omega} = -\frac{v_F^2}{2}\frac{\omega_C}{({\tau_{\text{eff}}}^{-1} - i\omega)^2 + 4\omega_C^2}.$$



Typical Setup



Experiment result in GaAs/GaAlAs



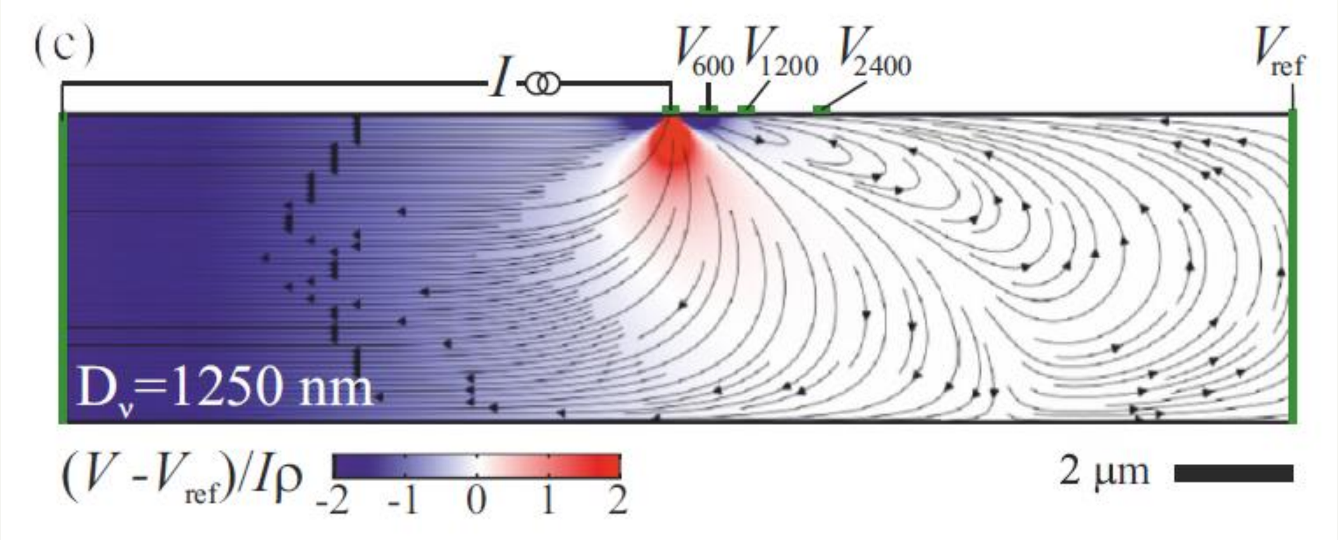
Theoretical result

$$\frac{\partial \boldsymbol{V}}{\partial t} = \eta_{xx}\Delta\boldsymbol{V} + [(\eta_{xy}\Delta\boldsymbol{V} + \omega_c\boldsymbol{V}) \times \boldsymbol{e}_z] + \frac{e}{m}(\boldsymbol{E} + \boldsymbol{V}\times\boldsymbol{B}) - \frac{\boldsymbol{V}}{\tau}$$

[1] Guo Y (郭洋裕). *Doctor Dissertation*. Tsinghua University, 2018.
[2] Huang Y (黄云帆). *Undergraduate Thesis*. Tsinghua University, 2019.

Conclusions

- **Electron and phonon hydrodynamics are possible** under certain circumstances, besides molecular hydrodynamics (fluid dynamics)**.**
- **Parallel treatment of the hydrodynamic transport is feasible** and will help predict and study the novel phenomena, i.e. Knudsen-Gurzhi effect.
- **Applications in scientific research and industry are expected** based on those hydrodynamic phenomena equipped with the theoretical framework.



Thank you!

Any comments are welcome!

Yunfan Huang

Department of Engineering Mechanics

yf-huang19@mails.tsinghua.edu.cn