

**2.57 Nano-to-Macro Transport Processes**  
**Fall 2004**  
**Lecture 18**

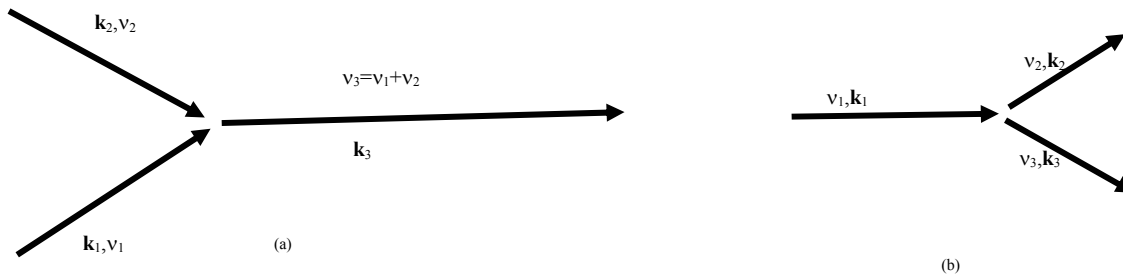
In last lecture, we deal with the Boltzmann transport equation

$$\frac{\partial f}{\partial t} + \frac{d\mathbf{r}}{dt} \cdot \nabla_{\mathbf{r}} f + \frac{d\mathbf{p}}{dt} \cdot \nabla_{\mathbf{p}} f = \left( \frac{\partial f}{\partial t} \right)_s$$

where the subscripts (**r** and **p**) in the gradient operators represent the variables of the gradient. The scattering term  $\left( \frac{\partial f}{\partial t} \right)_s = -\frac{f - f_0}{\tau}$  was discussed based on two particle interactions. Here  $\tau(\omega, \mathbf{k})$  is the relaxation time. For equilibrium distribution  $f_0$ , we have

$$f_0 = \begin{cases} \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1} & \text{Bose-Einstein distribution (phonon)} \\ \frac{1}{e^{\frac{E-\mu}{k_B T}} + 1} & \text{Fermi-Dirac distribution (electron)} \\ n \left( \frac{m}{2\pi k_B T} \right)^{3/2} e^{-\frac{m|\mathbf{v}-\mathbf{u}|^2}{2k_B T}} & \text{Displaced Maxwell velocity distribution (molecules)} \end{cases}$$

Note: The relaxation time is due to combined factors and can be evaluated numerically by adding all possible influence together. This idea can be used in calculating the band structure by the Boltzmann transport equation.



For two-particle interactions (above figure (a)), we have

$$\hbar\omega_1 + \hbar\omega_2 = \hbar\omega_3 \quad (\text{energy conservation}),$$

$$\mathbf{G} + \mathbf{k}_3 = \mathbf{k}_1 + \mathbf{k}_2 \quad (\text{momentum conservation}),$$

where zero **G** corresponds to normal process, otherwise it is umklapp scattering.

Generally speaking, electrons will collide with electrons, phonons, and impurities in the crystals. The electron-phonon scattering causes the electrical resistance.

Note: At low temperatures, phonon has low energy and the electron-phonon scattering is negligible. Therefore, the impurity-electron scattering is the main cause of electrical resistance.

For gas molecules, in Lecture 2 we have derived the collision obeys

$$\Lambda = \frac{1}{\sqrt{2n\pi D^2}}, \quad \Lambda = \bar{v}\tau.$$

Note: (1) To simplify, most time we view  $\tau(\omega, \mathbf{k})$  as  $\tau(\omega)$ . (2) The time  $\tau(\omega, \mathbf{k})$  is only applicable to elastic scattering (see chapter 8), such as electron-electron scattering (energy conserved). It is not accurate for electron-phonon scattering. In this situation, we have  $\left(\frac{\partial f}{\partial t}\right)_s = -\frac{f - f_0}{\tau} + g(T_e - T_p)$ . (3) In semiconductor devices,  $T_e$  can be thousands of degrees, while  $T_p$  is only hundreds degrees. The two temperatures differ a lot.

We can understand the meaning of  $\tau$  easily by neglecting the spatial non-uniformity of the distribution function. The Boltzmann transport equation becomes

$$\frac{\partial f}{\partial t} = -\frac{f - f_0}{\tau}$$

and thus

$$f - f_0 = C e^{-t/\tau}$$

So the relaxation time is a measure of how long it takes for a nonequilibrium system to relax back to an equilibrium distribution.

Consider the Boltzmann equation under the relaxation time approximation. Let's introduce a deviation function  $g$ ,

$$g = f - f_0$$

and write the Boltzmann equation as

$$\frac{\partial g}{\partial t} + \frac{\partial f_0}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f_0 + \mathbf{v} \cdot \nabla_{\mathbf{r}} g + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} f_0 + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} g = -\frac{g}{\tau}$$

Note:  $\nabla_{\mathbf{p}} f = \frac{1}{\hbar} \nabla_{\mathbf{k}} f = \frac{1}{m} \nabla_{\mathbf{v}} f$ . We can also express  $f(t, \mathbf{r}, \mathbf{p})$  as  $f(t, \mathbf{r}, \mathbf{v})$  or  $f(t, \mathbf{r}, \mathbf{k})$  for convenience.

All the diffusion laws can be obtained under the following assumptions (1) the transient terms are negligible, (2) the gradient of  $g$  is much smaller than the gradient of  $f_0$ , and similarly,  $g$  is much smaller than  $f_0$ . Under these assumptions, the above equation becomes

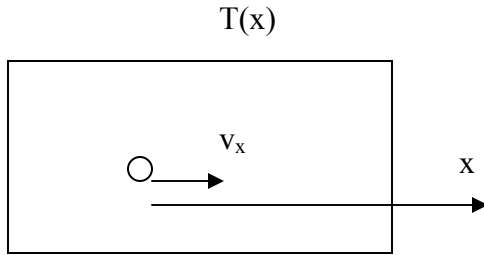
$$g = -\tau \left( \mathbf{v} \cdot \nabla_{\mathbf{r}} f_0 + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} f_0 \right)$$

or

$$f = f_o - \tau \left( \mathbf{v} \cdot \nabla_{\mathbf{r}} f_o + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} f_o \right).$$

From the distribution function changing in long period compared with the relaxation time, we can calculate the flux of various quantities of interests (charge, momentum, and energy).

Fourier Law



For simplicity, we consider a temperature gradient along the x-direction without loss of generality. We can calculate the heat flux from

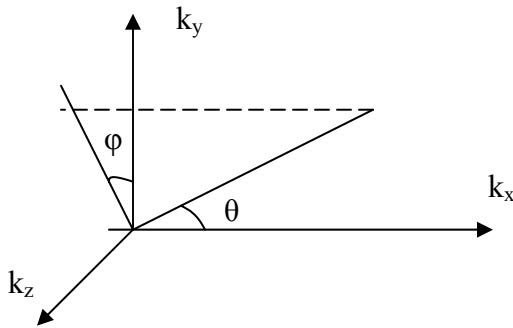
$$J_{qx}(x) = \sum_p \left[ \frac{1}{V} \sum_{k_{x1}=-\infty}^{\infty} \sum_{k_{y1}=-\infty}^{\infty} \sum_{k_{z1}=-\infty}^{\infty} v_x \hbar \omega(\omega) f \right]$$

where p represents the summation over all polarizations. It is interesting to compare this expression with what we used in deriving the Landauer formalism. In that equation, we are considering only the heat flux going from point 1 to point 2 and there also exists a reverse heat flux from point 2 to point 1. Here we are considering the net heat flux at any constant x-plane inside the domain.

As in previous lectures, we can convert the summation into integral and further change into spherical coordinates

$$J_{qx}(x) = (1/V) \sum_p \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} v_x \hbar \omega f dk_x dk_y dk_z / (2\pi/L)^3$$

$$= \int_0^{\omega_{\max}} d\omega \left[ \int_0^{2\pi} \left\{ \int_0^{\pi} v \cos \theta \hbar \omega f \frac{D(\omega)}{4\pi} \sin \theta d\theta \right\} d\varphi \right]$$



Note: Here theta varies from 0 to pi because both positive and negative v\_x are considered.

With  $f = f_o - \tau \left( \mathbf{v} \cdot \nabla_{\mathbf{r}} f_o + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} f_o \right)$ , we obtain

$$\begin{aligned}
 J_{qx}(x) &= \int_0^{\omega_{\max}} d\omega \left[ \int_0^{2\pi} \left\{ \int_0^{\pi} v \cos \theta \hbar \omega \left[ f_o - \tau \frac{df_o}{dT} \frac{dT}{dx} v \cos \theta \right] \frac{D(\omega)}{4\pi} \sin \theta d\theta \right\} d\varphi \right] \\
 &= -\frac{1}{2} \frac{dT}{dx} \int_0^{\omega_{\max}} d\omega \left\{ \int_0^{\pi} \tau v^2 \sin \theta \cos^2 \theta \times \hbar \omega D(\omega) \frac{df_o}{dT} d\theta \right\} \\
 &= -\frac{1}{3} \frac{dT}{dx} \int_0^{\omega_{\max}} d\omega \left\{ \int_0^{\pi} \tau v^2 \frac{d(\hbar \omega D(\omega) f_o)}{dT} d\theta \right\} \\
 &= -\frac{1}{3} \frac{dT}{dx} \int_0^{\omega_{\max}} d\omega \left\{ \int_0^{\pi} \tau v^2 C(\omega) d\theta \right\}
 \end{aligned}$$

and

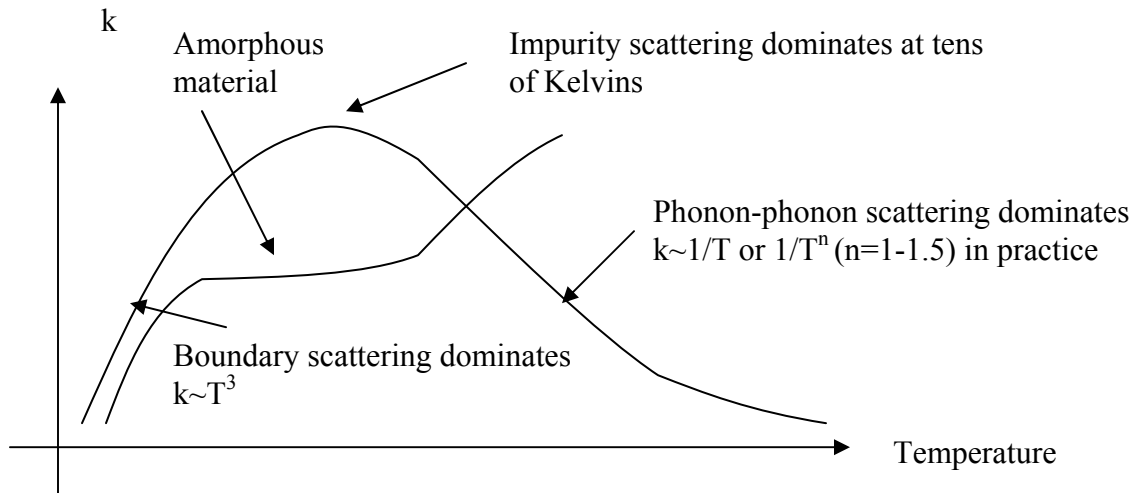
$$k = \frac{1}{3} \int \tau v^2 C d\omega \text{ in the Fourier law.}$$

Note: The equilibrium  $f_o$  term drops out in the integral, which is consistent with our expectation.

In the case that both  $\tau$  and  $v$  (group velocity  $v = d\omega/dk$ ) are independent of frequency, the above expression recover to the kinetic relation

$$k = \frac{1}{3} C v \Lambda.$$

The temperature-dependent thermal conductivity for a material is drawn in the following figure. For amorphous materials, two transition points exist.

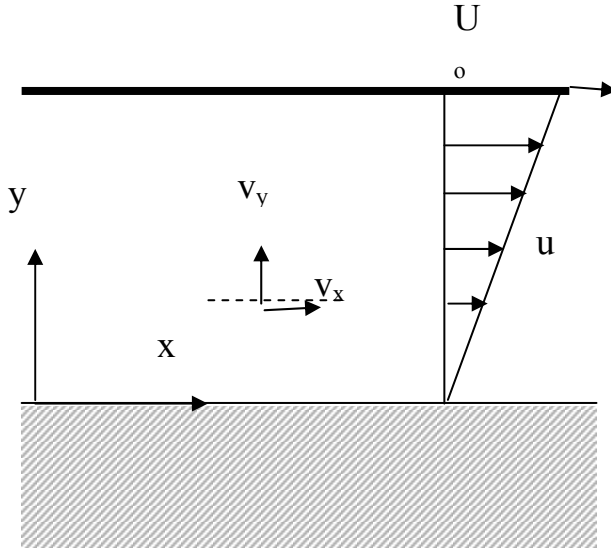


Newton's Shear Stress Law

In the following figure, a couette flow is shown. As an approximation, the following **displaced Maxwell velocity distribution** is often used for the probability of finding one particle having velocity  $\mathbf{v}$

$$P(v_x, v_y, v_z) = \left( \frac{m}{2\pi\kappa_B T} \right)^{3/2} e^{-m \left[ (v_x - u)^2 + v_y^2 + v_z^2 \right] / 2\kappa_B T}$$

where  $u$  is the average velocity along the x-direction (spatially changed).



Assuming that the number density of particles is  $n$ , the number density of particles having velocity  $\mathbf{v}$  is

$$f_0(v_x, v_y, v_z) = n P(v_x, v_y, v_z) = n \left( \frac{m}{2\pi\kappa_B T} \right)^{3/2} e^{-m \left[ (v_x - u)^2 + v_y^2 + v_z^2 \right] / 2\kappa_B T}$$

From  $f = f_0 - \tau (\mathbf{v} \cdot \nabla_r f_0)$  ( $\mathbf{F}$  is zero because this is no external fields here and gravity is neglected), the distribution function is

$$f = f_0 - \tau (v_x \hat{i} + v_y \hat{j} + v_z \hat{k}) \cdot \left( \frac{\partial f_0}{\partial x} \hat{i} + \frac{\partial f_0}{\partial y} \hat{j} + \frac{\partial f_0}{\partial z} \hat{k} \right) = f_0 - \tau v_y \frac{\partial f_0}{\partial y} = f_0 - \tau v_y \frac{\partial f_0}{\partial u} \frac{\partial u}{\partial y}$$

Compared with the law  $\tau_{xy} = \mu \frac{\partial u}{\partial y}$  ( $x$  is the force direction,  $y$  is the normal direction), we

have

$$\mu = n\tau k_B T$$

Following a similar procedure, we can also calculate the energy flux due to molecular heat conduction and obtain the thermal conductivity for a gas as

$$k = \frac{5}{2} \left( \frac{k_B}{m} \right) n\tau k_B T = \frac{5}{2} \left( \frac{k_B}{m} \right) \mu$$

Note: The thermal conductivity and dynamic viscosity have similar form here because they are based on the same mechanism.

In the following lecture, we will discuss the Ohm's Law and Wiedmann-Franz's Law. The force acting on the electron by the external field is

$$\mathbf{F} = -e\mathbf{E},$$

where  $e$  is the unit charge, and the charge of an electron is  $(-e)$ ,  $\mathbf{E}$  is the electric field. And  $f_0$  obeys the Fermi-Dirac distribution

$$f_0(E, E_f, T) = \frac{1}{\exp\left(\frac{E - E_f}{\kappa_B T}\right) + 1}.$$

We will deal with  $\mu$ ,  $T$  and  $F$  simultaneously in this situation.