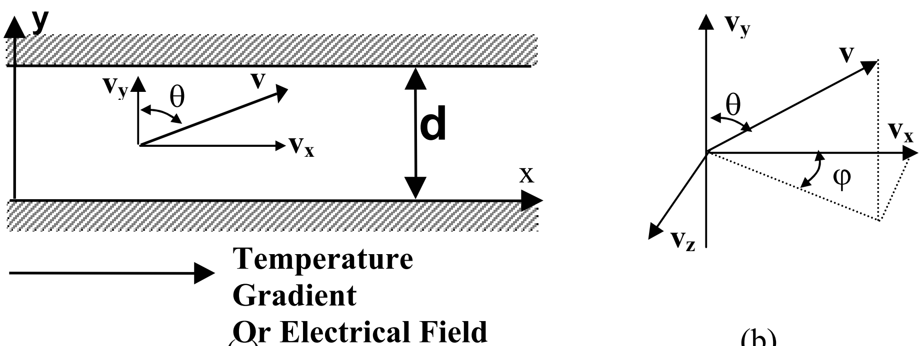
2.57 Nano-to-Macro Transport Processes
Fall 2004
Lecture 22

We have talked about the heat flux as

$$q_x = \frac{1}{V}\sum_{k_x}\sum_{k_y}\sum_{k_z} f v_x \hbar\omega .$$



(a) (b)

The Boltzmann equation is

$$\tau\vec{v}\cdot\nabla_{\vec{r}} g + g = -\tau\left(\vec{v}\cdot\nabla_{\vec{r}} f_0 + \frac{\vec{F}}{m}\cdot\nabla_{\vec{v}} f_0\right) = S_0 ,$$

where $\frac{\vec{F}}{m}\cdot\nabla_{\vec{v}} f_0 = 0$ for phonons, g=f-f_0. Noticing $\vec{v}\cdot\nabla_{\vec{r}} g \approx v_y \frac{\partial g}{\partial y}$ (d<<x) and $\nabla_{\vec{r}} f_0 = \frac{df_0}{dT}\frac{dT}{dx}$, the x direction component gives

$$g + \tau v_y \frac{\partial g}{\partial y} = -\tau v_x \frac{df_0}{dT}\frac{dT}{dx} = S_0(x),$$

the solution of which is

$$g - S_0 = C\exp\left(-\frac{y}{v_y\tau}\right).$$

One boundary condition is required to determine C.

Assuming both top and bottom of the film diffusely scatter phonons, we have

$$\begin{cases} y = 0, f = f_0, g = 0 \text{ for } \theta \in \left(0, \frac{\pi}{2}\right) \\ y = d, f = f_0, g = 0 \text{ for } \theta \in \left(\frac{\pi}{2}, \pi\right) \end{cases}.$$

Finally we get

At y = 0, $\theta \in \left(0, \frac{\pi}{2}\right)$, C = -$S_0$, $g(y,\theta) = S_0\left(1 - \exp\left(-\frac{y}{v\tau\cos\theta}\right)\right)$, At y = d, $\theta \in \left(\frac{\pi}{2}, \pi\right)$, C = -$S_0 \exp\left(d / v\tau\cos\theta\right)$, $g\left(y,\theta\right) = S_0\left(1-\exp\left(\frac{d-y}{v\tau\cos\theta}\right)\right)$.

Note: $\frac{y}{v\tau\cos\theta}$ is the ratio between the traveled distance and the mean free path of phonons.

$$q_x\left(y\right) = \frac{1}{V}\sum_{v_x}\sum_{v_y}\sum_{v_z}\hbar\omega v_x f = \int_0^{\omega_{\max}} d\omega \int_0^{2\pi} d\varphi \int_0^{\pi} \hbar\omega v_x f \frac{D(\omega)}{4\pi}\sin\theta d\theta,$$

where $v_x = v\sin\theta\cos\varphi$ according to our spherical coordinate system, f=g+f_0. Thus

$$q_x\left(y\right) = \int_0^{\omega_{\max}} d\omega \int_0^{2\pi} d\varphi [\int_0^{\frac{\pi}{2}} \hbar\omega\left(v\cos\varphi\sin\theta\right)\left(-\tau v\cos\varphi\sin\theta\frac{df_0}{dT}\frac{dT}{dx}\left(\exp\left(-\frac{y}{v\tau\cos\theta}\right)-1\right)\right)\frac{D(\omega)}{4\pi}\sin\theta d\theta +$$

$$\int_{\frac{\pi}{2}}^{\pi} \hbar\omega\left(v\cos\varphi\sin\theta\right)\left(-\tau v\cos\varphi\sin\theta\frac{df_0}{dT}\frac{dT}{dx}\left(\exp\left(\frac{d-y}{v\tau\cos\theta}\right)-1\right)\right)\frac{D(\omega)}{4\pi}\sin\theta d\theta]$$

Note: At y=0, the x-direction heat flux is nonzero. In the above expression, the second integral is not zero though the first one is.

Now let $\cos\theta = \mu$ and thus $\sin\theta d\theta = -d\mu, \sin^3\theta d\theta = -\left(1-\mu^2\right)d\mu$. Also define $E_n\left(\xi\right) = \int_0^1 \mu^{n-2}\exp\left(-\frac{\xi}{\mu}\right)d\mu$, $\xi = \frac{d}{\Lambda}, \Lambda = \tau v$. Noting $\int_0^{2\pi}\cos^2\varphi d\varphi = \pi$, the total heat flow per unit width is

$$Q = \int_0^d q\left(y\right)dy$$

$$= -\frac{\pi}{4}\frac{dT}{dx}\int_0^{\omega_{\max}} \hbar\omega\frac{df_0}{dT}\tau v^2 D\left(\omega\right)d\omega\ [\int_0^1\left(1-\mu^2\right)d\mu\left(\Lambda\mu\left(\exp\left(-\frac{\xi}{\mu}\right)-1\right)-d\right)+$$

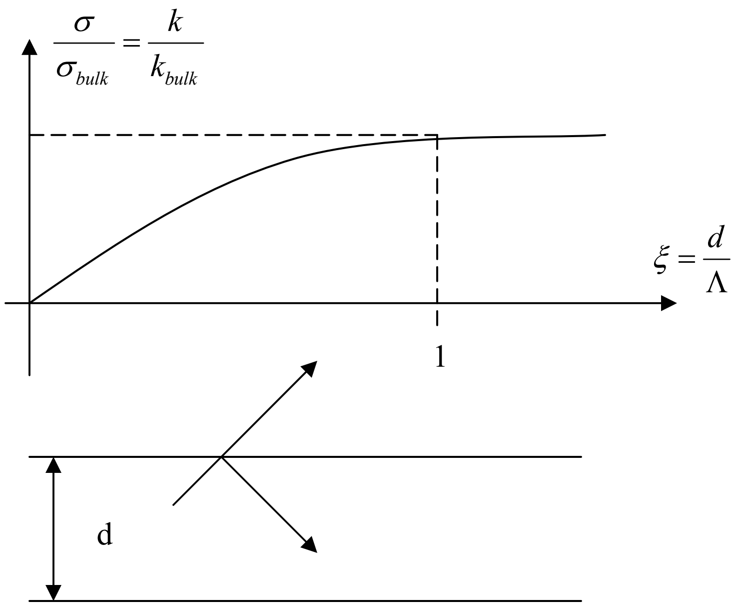
$$\int_0^1\left(1-\mu^2\right)d\mu\left(-\Lambda\mu\left(1-\exp\left(-\frac{\xi}{\mu}\right)\right)-d\right)]$$

$$= -kd\frac{dT}{dx},$$

which yields (if Λ is independent on ω)

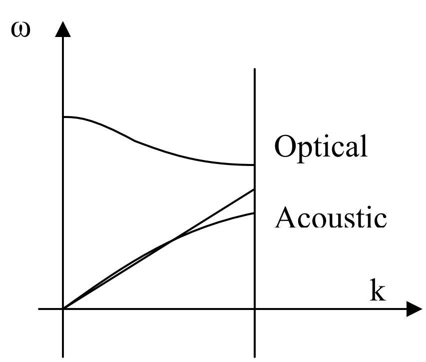
$$k / k_{bulk} = 1 - \frac{3}{8\xi}\left(1-4E_3\left(\xi\right)-E_5\left(\xi\right)\right).$$

The tendency is drawn in the following figure. It is expected that k approaches the bulk value for d larger than the mean free path. Since in diffuse scattering part of the phonons are scattered backward, the loss of x-direction momentum results in a lower thermal conductivity.



For specular case (above figure), the x-direction momentum is conserved. Following all these procedures, we can finally prove $k=k_{bulk}$.

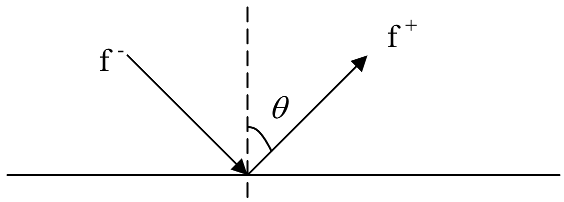
Note: To determine the mean free path, we should use $k = \frac{\overline{\Lambda}}{3}\int C_\omega v_\omega d\omega$ instead of the simplified $k = \frac{Cv\Lambda}{3}$, which gives an underestimation of Λ. This is because the Debye approximation overestimates the velocity approach the edge of the first Brillouin zone, where the group velocity should be zero.



For partial specular (momentum conserved) and partial diffuse (momentum not conserved), we have

$f^+(\mu,0) = pf^-(-\mu,0) + 2(1-p)\int_0^1 f^-(-\mu,0)\mu d\mu$,

where p represents the ratio of specular scattering.



Now consider the y direction. Similarly, we have

$$\tau v_y \frac{\partial g}{\partial y} + g = -\tau v_y \frac{df_0}{dT}\frac{dT}{dy} = S_0(y).$$

To solve this, first let $S_0(y)$=0, then $g = C\exp\left(-\frac{y}{\tau v_y}\right)$. In general, use $C(y)$ to replace C. Substitute into the governing equation, we get

$$\tau v_y \exp\left(-\frac{y}{\tau v_y}\right)\frac{dC}{dy} = S_0(y),$$

$$C = \int_y^{y_0} S_0(y')\frac{\exp\left(\frac{y'}{\tau v_y}\right)}{\tau v_y}dy' + C(y_0),$$

$$g(y) = C(y_0)\exp\left(-\frac{y}{\tau v\cos\theta}\right) + \int_y^{y_0} S_0(y')\frac{\exp\left(\frac{y'-y}{\tau v_y}\right)}{\tau v_y}dy'.$$

Now the boundary condition is (elastic scattering on boundaries)

$$\begin{cases} y = 0, f = f_0, g = 0, C(0) = 0 \text{ for } \theta \in \left(0, \frac{\pi}{2}\right) \\ y = d, f = f_0, g = 0, C(d) = 0 \text{ for } \theta \in \left(\frac{\pi}{2}, \pi\right) \end{cases}.$$

At steady state, we have

$$Const = q_y = \int_0^{\omega_{\max}} \hbar\omega d\omega \int_0^{2\pi} d\varphi \int_0^{\pi} v_y f \frac{D(\omega)}{4\pi} d\theta$$

And $\frac{dq_y}{dy} = 0$ yields

$$2\theta(\eta) = E_2(\eta) + \int_0^{\xi} \theta(\eta')E_1(|\eta - \eta'|)d\eta'$$

where we used dimensionless parameters $\theta(y) = \frac{T_1(y) - T_2}{T_1 - T_2}, \eta = \frac{y}{\Lambda}, \xi = \frac{d}{\Lambda}$.

The temperature profiles for two extreme cases are drawn in the following figure. For $\xi \to 0$ (note $T_1 \neq T_2$), it is in nonequilibrium state but we define the equilibrium conception, temperature, based on the average value.