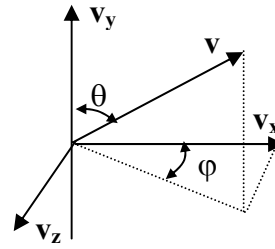
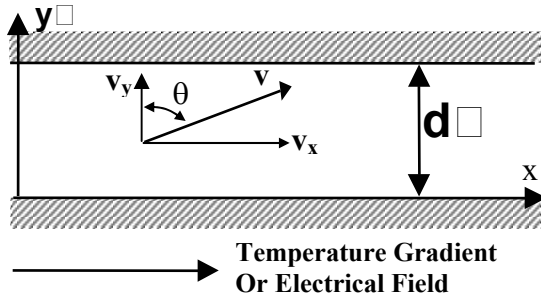


2.57 Nano-to-Macro Transport Processes
Fall 2004
Lecture 23

In the last lecture, we talked about the energy flux along a thin film as

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



Now let us consider the conduction of gas molecules between two plates. Similarly, the Boltzmann equation is

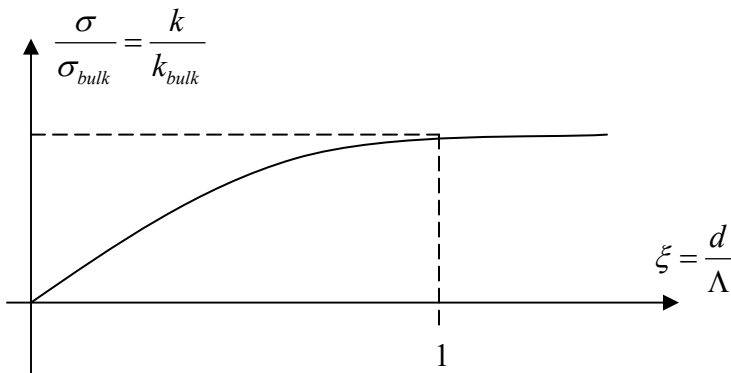
$$\tau \vec{v} \cdot \nabla_r g + g = -\tau \left(\vec{v} \cdot \nabla_r f_0 + \frac{\vec{F}}{m} \cdot \nabla_v f_0 \right),$$

where the bulk force $\frac{\vec{F}}{m} \cdot \nabla_v f_0 = 0$ for phonons, $g = f - f_0$. Noticing $\vec{v} \cdot \nabla_r g \approx v_y \frac{\partial g}{\partial y}$ ($d \ll x$)

and $\nabla_r f_0 = \frac{df_0}{dT} \frac{dT}{dx}$, the x direction component gives

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

We can solve g first and then substitute the expression $f = g + f_0$ into any flux equation. Under the diffuse assumption, we obtain the following figure for the conductivities of the material.



In the y direction, we have

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

Since no heat is generated in the volume, we finally obtain $q(y) = \text{const}$. The

normalized temperature $\theta(\eta) = \frac{T(\eta) - T_2}{T_1 - T_2}$ obeys

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

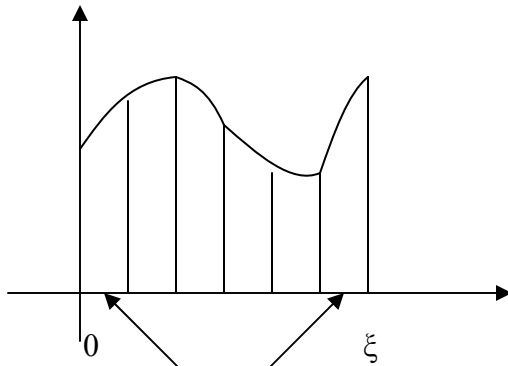
where $\eta = y/\lambda$, $\xi = d/\lambda$, $\lambda/d = \text{Knudsen number}$, $\theta(\eta)$ may also represent normalized

blackbody emissive power $\frac{u(y) - u_2}{u_1 - u_2} = \frac{T^4(y) - T_2^4}{T_1^4 - T_2^4}$. This is the linear, nonhomogeneous,

Fredholm integral equation of the second kind. The function $E_1(|\eta - \eta'|)$ is called the kernel. The Fredholm integral equation does not have an analytical solution, although approximate solution methods have been developed.

To solve the equation numerically, first we discretize the equation with

$$\frac{d^2 T}{dx^2} = \frac{T_{i+1} - 2T_i + T_{i-1}}{2\Delta x^2}.$$



Half trapezium at both ends

The integration is calculated by dividing the area into many trapezia. We have

$$\int_0^\xi \theta(\eta') E_1(|\eta - \eta'|) d\eta' = \theta(0) \frac{E_1(\eta)}{2} \Delta\eta + \theta(\xi) \frac{E_1(\xi - \eta)}{2} \Delta\eta + \Delta\eta \sum_1^{n-1} \theta(\eta_i) E_1(|\eta - \eta_i|),$$

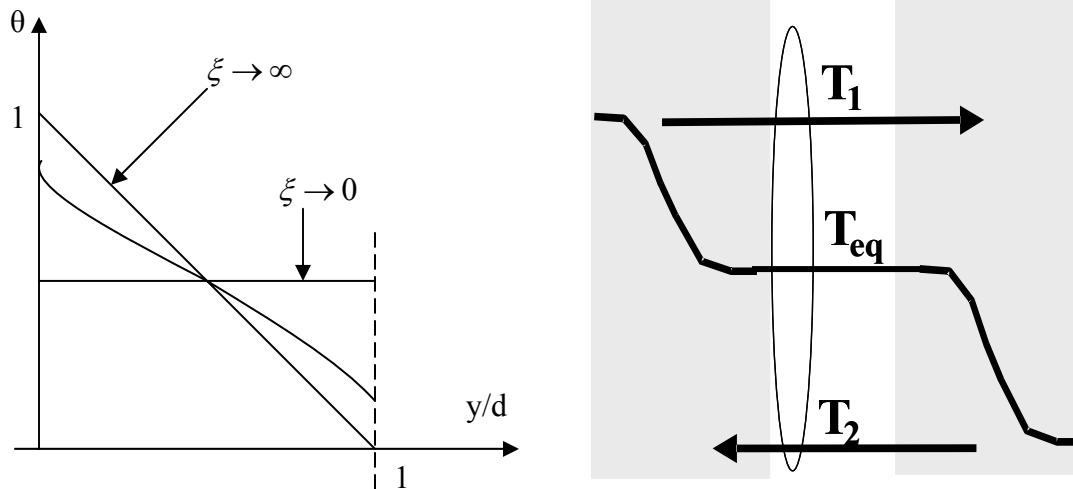
which gives totally $n+1$ equations (n is the section number). Therefore, we get a set of linear equations for $\theta(\eta_i)$ to solve.

Another way to conduct the integration is to use the Gauss- Legendre method, which

generates sections in $(0, \xi)$ with varying width. Then we can use $\int_0^1 f(x) dx = \sum_{i=1}^n f(x_i) W_i$

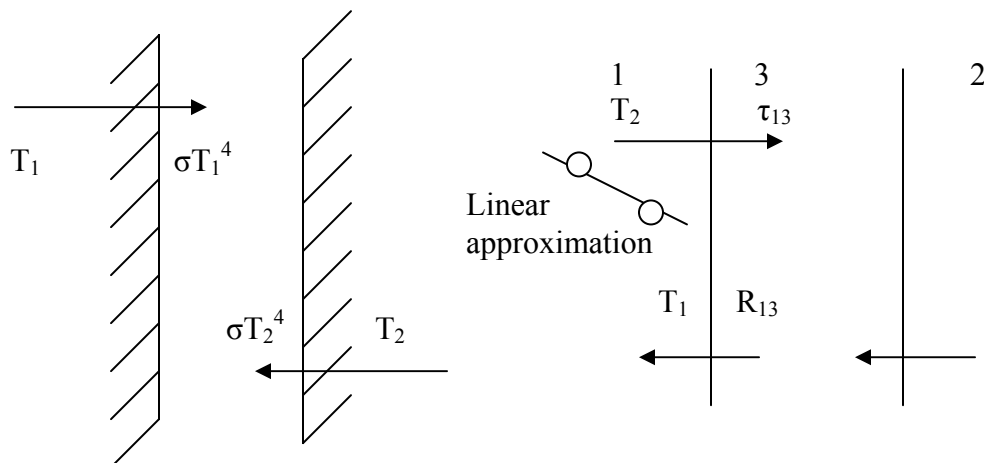
to find the approximating value, where W_i is the weight of different $f(x_i)$.

The temperature $\theta(\eta) = \frac{T(\eta) - T_2}{T_1 - T_2}$ within d is shown as following, which was discussed in the last lecture. When $\xi = d/\lambda \rightarrow 0$, $T(y) = \frac{T_1 + T_2}{2}$.

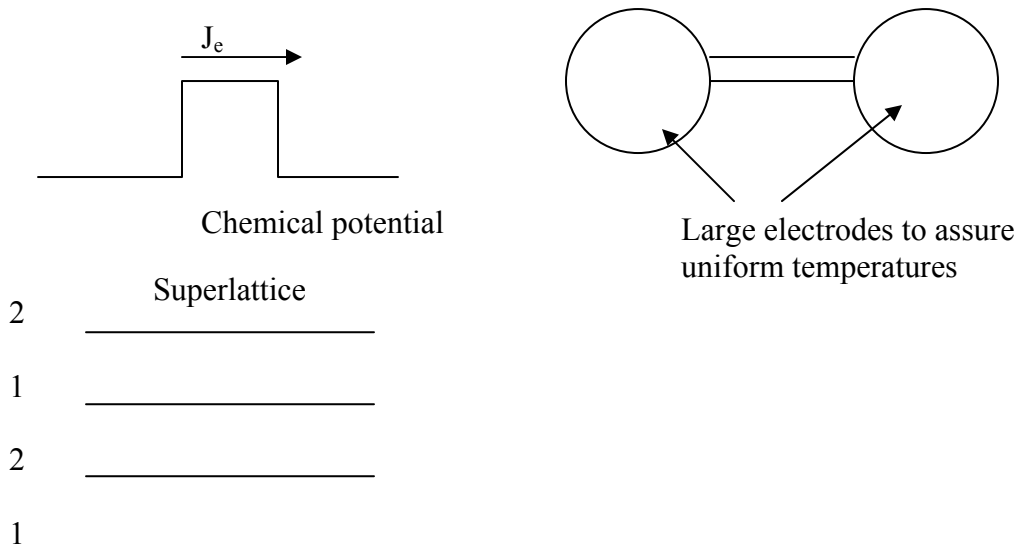


More generally, θ should be the internal energy of the carriers. For photons, $\theta(y) = \frac{u(y) - u_2}{u_1 - u_2} = \frac{T^4(y) - T_2^4}{T_1^4 - T_2^4}$.

The interpretation of the temperature discontinuity is worthy of special attentions. Sometimes, the jump is physical, while in other cases the jump is artificial. The discontinuity arises from the boundary conditions. We assume the boundaries are diffuse and carriers coming into the region are at temperatures T_1 and T_2 (emitted temperatures). These temperatures represent only those carriers entering the thin film. For photon transport, these are good representations of the carriers coming into the region because the internal conduction in both walls is much stronger and determines the solid temperatures that emit the photons. In this case, the temperature jump represents the difference of the solid temperature and the photon temperature inside the film.

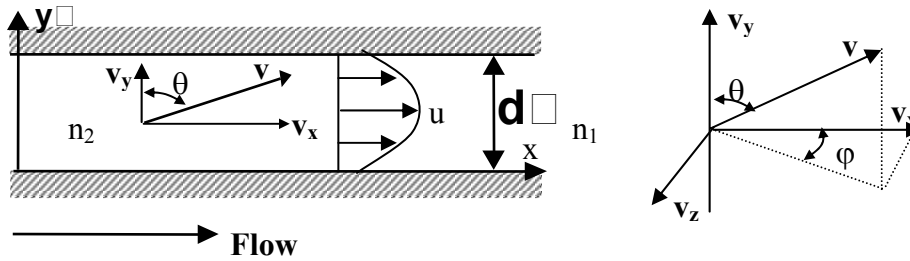


For phonons, if the walls are assumed to be black, it also means that transmissivity equals one and there exists no thermal boundary resistance. The phonon temperature inside region 1 should equal to that temperature in the film at the boundary. The temperature jump is artificial, and arises from the fact T_1 and T_2 are only emitted phonon temperature entering the thin film, not the local equilibrium temperature as we use in the Fourier law or solved directly from the Boltzmann equation. However, if the interface reflectivity is not zero, there exists a temperature jump just as in the case of thermal boundary resistance that we discussed in chapter 5. The value of this temperature jump is different from what is given from the boundary condition used. This issue related to consistent use of a definition for temperature was also discussed for the case of thermal boundary resistance. Many comparisons between experimental data and theory are based on inconsistent definition on temperature and are thus wrong (theoretically). In heat conduction experiments, one usually measure two points close to the interface and use linear approximation to get the temperatures on both sides of the interface. The temperature obtained is consistent with the Fourier law but not consistent with the boundary conditions we use here in the solution of the Boltzmann equation. Iterative procedures are needed if one want to modify the boundary condition to be consistent with the temperatures defined in the Boltzmann equation and the Fourier law. Similar phenomena also happen in when dealing with electron transport across an interface. Most people use drift-diffusion equations up to the interface and use Richardson formula (which is based on the emitted electron properties including their chemical potential and temperature). There are cases, however, one measure the emitted electron and phonon temperature or chemical potential, as in the case of photon radiation discussed above. One example is in the experiment determining the quantized conductance of a nanowire. The electrodes are large and the measured voltage drop should represent the differences of electrons entering the channel.

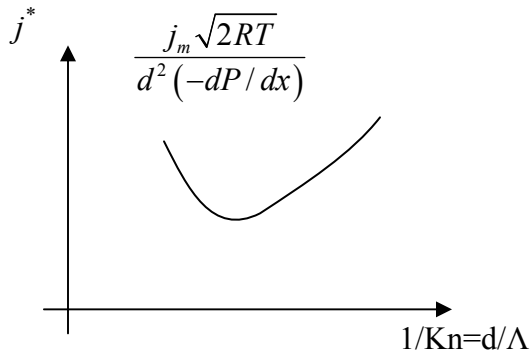


I found the importance of a consistent usage of the temperature definition when dealing with heat conduction in superlattices. For the above superlattice case, a consistent

temperature definition must be used such that results from Boltzmann equation and from simple ray tracing in the limit of no scattering agrees with each other.

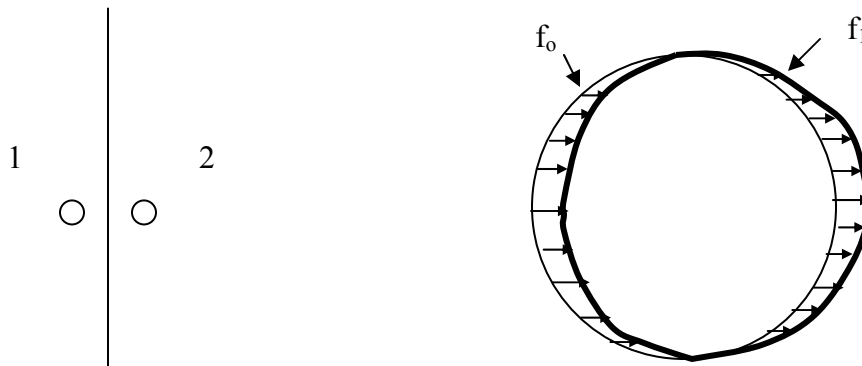


For gas flow through two plates (driven by pressure difference), the velocity has a drop on the surface, which is called slip boundary condition. The mass flow rate per unit depth is drawn in the following figure. The mass flow rate demonstrates the existence of the Knudsen minimum around $K_n=1$ and is in reasonably good agreement with experimental results of Dong (1956).



Now let us consider the interface temperature drop with learned equations. Here we use diffusion approximation inside ($\vec{v} \cdot \nabla_{\vec{r}} g$ is dropped in Boltzmann equation), and assume diffusion/transmission boundary conditions. The Boltzmann equation becomes

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



In the above left figure, at the interface we have

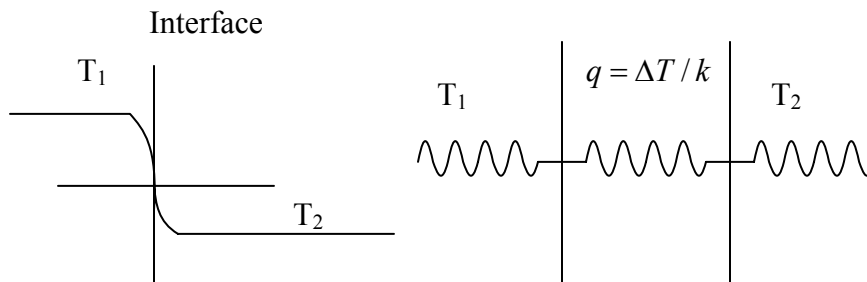
$$q = \sum_{v_{x1} > 0, v_{y1}, v_{z1}} \tau_{12} \hbar \omega v_{x1} f_1 + \sum_{v_{x2} > 0, v_{y2}, v_{z2}} \tau_{21} \hbar \omega v_{x2} f_2.$$

Note in the right figure, only rightward arrows indicate transport to the second region ($V_x > 0$). Define τ_{12}' , τ_{21}' as the average transmissivity in each region. We have

$$q = \sum_{v_{x1} > 0, v_{y1}, v_{z1}} \tau_{12} \hbar \omega v_{x1} f_{01} + \sum_{v_{x2} > 0, v_{y2}, v_{z2}} \tau_{21} \hbar \omega v_{x2} f_{02} + \tau_{21}' \frac{q}{2} + \tau_{12}' \frac{q}{2},$$

$$\left[1 - \frac{1}{2}(\tau_{21}' + \tau_{12}')\right] q = \sum_{v_{x1} > 0, v_{y1}, v_{z1}} \tau_{12} \hbar \omega v_{x1} [f_{01}(T_1) - f_{02}(T_2)].$$

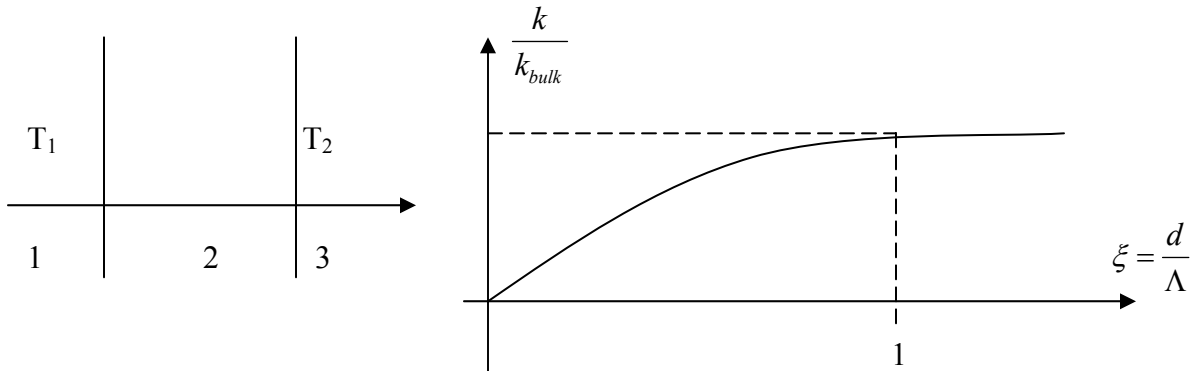
If $\tau_{21}' = \tau_{12}' = 1$, no temperature drop happens in the above relationship. In practice, τ_{21}' , τ_{12}' are difficult to determine.



For the case drawing as below, we have

$$\frac{k_{eff}}{k_{bulk}} = \frac{3d/4\Lambda}{\frac{1 - \frac{1}{2}(\tau_{12}' + \tau_{21}')}{\tau_{21}''} + \frac{1 - \frac{1}{2}(\tau_{23}' + \tau_{22}')}{\tau_{23}''} + 3d/4\Lambda},$$

where $3d/4\Lambda \ll \frac{1 - \frac{1}{2}(\tau_{12}' + \tau_{21}')}{\tau_{21}'} + \frac{1 - \frac{1}{2}(\tau_{23}' + \tau_{22}')}{\tau_{23}'}$ in thin films, while in bulk materials $3d/4\Lambda$ is dominant. We have similar relationship as previous cases.



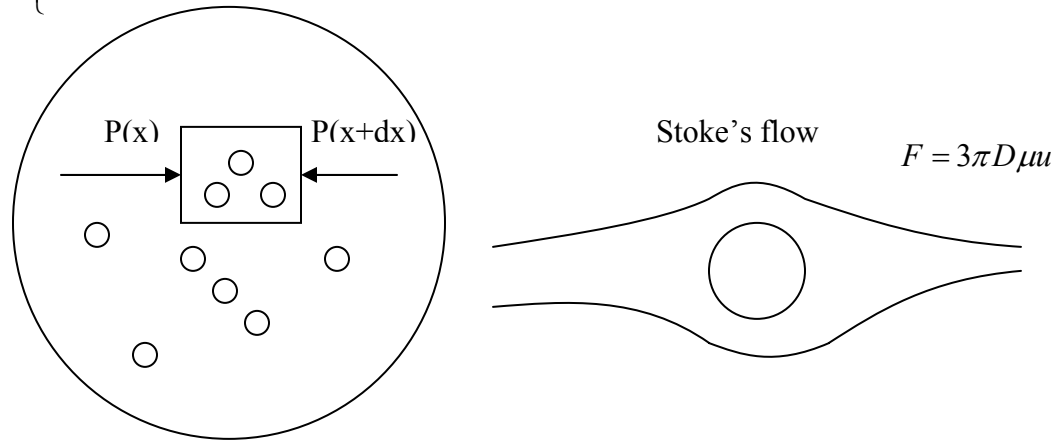
Chapter 9 Liquids

For gases, after two particles collide, they do not have any memory of previous history. However, this is not true for solids and liquids, in which their previous locations affect

the shape change. The Boltzmann equation is only applicable to diluted gases. To deal with liquids, other approaches must be used. We list some of the efforts in this aspect.

Approaches {

- Modified Boltzmann equation {
 - Two-particle distribution function
 - Enskog equation (denser gases)
- Einstein (Brownian motion) \Rightarrow Langerin equation \Rightarrow
- Linear response theory \Rightarrow Molecular Dynamics



In the left figure above, pressure difference exists in the fluid. For one particle, the osmotic pressure is determined by

$$P = \frac{1}{V} Nk_B T = nk_B T .$$

Also, we can use the solution of Stoke's flow around a sphere. The force is $F = 3\pi D\mu u$.