5.1 Heat conduction

In last lecture, we describe electrons as free electron gas and lattice vibrations as phonon gas. Basically they are both gases in a box.

5.2 Convection
1) Typically electron velocities are 10^5-10^6 m/s, while phonon velocities are the sound velocity.
2) In heat conduction processes, the average velocity of heat carriers is $\bar{\bar{v}} = 0$. In convection, a non-vanishing average velocity superimposed on their random velocity, resulting in $\bar{\bar{v}} \neq 0$.
3) When a liquid or gas molecule is moved from one place to another due to its nonzero velocity, it also carries its internal energy.
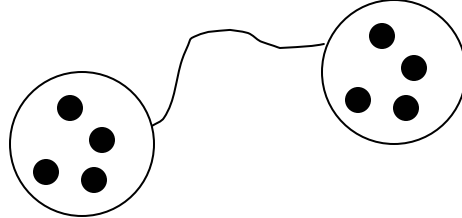

5.3 Radiation
1) Wavelength comparison
   For radio/TV signals, we get
 $$\lambda = c/f = \frac{3 \times 10^8}{900 \times 10^6} = \frac{1}{3} \text{ (m)},$$
   where we use 900 MHz as the frequency. This wavelength is still much larger than that of the thermal radiation (around 0.5 μm).
2) Generation of thermal radiation
   Thermal radiation typically refers to the electromagnetic waves that are generated by the oscillation charges in the atoms and crystals, while TV and radio signals are generated by artificial current oscillation in a circuit. An electromagnetic wave at frequency ν can only have energy that is multiple times of $h\nu$.
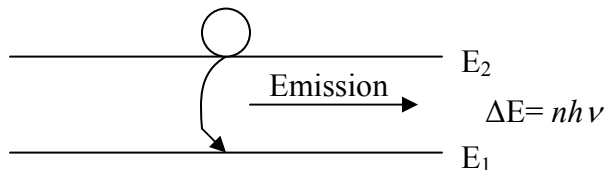
5.4 Pressure and shear stress
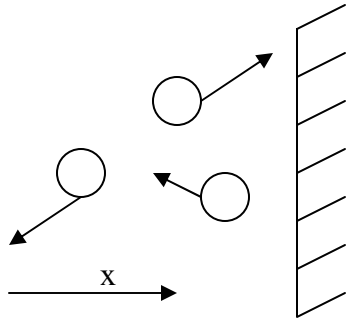
    As is shown in the figure, the velocities of gas molecules distribute randomly in all directions. Pressure is caused by their momentum changes normal to the wall. For one molecule, we have

$$\vec{F} = m\vec{a} = \frac{d(m\vec{v})}{dt} \text{ or } F_x = \frac{m(v_{x>0} - v_{x<0})}{\Delta t} = \frac{m\Delta v_x}{\Delta t}.$$

Denote n [m^{-3}] as the number of particles per unit volume. We notice nv_x [m^{-2}s^{-1}] has the physical meaning as the flux of particles on the wall. Assuming elastic collisions between the wall and molecules, we have $\Delta v_x = 2v_{x>0}$. Thus

$$P = \frac{1}{2}nv_{x>0}(m\Delta v_x) = mnv_{x>0}^2 = mnv_x^2 = mn\frac{v^2}{3},$$

in which we use average $v^2 = v_x^2 + v_y^2 + v_z^2 = 3v_x^2$. From here, you can derive the ideal gas law using the relationship between velocity and temperature that I will talk below.

    For assignment 1, similar processes can be followed to calculate the shear stress.
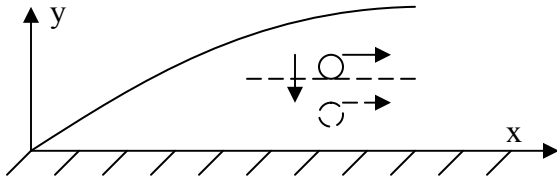
5.5 Charge transport
Similarly, we have

$$\vec{F} = q\vec{\varepsilon} = -e\vec{\varepsilon} \ ; \ \vec{J} = \sigma\vec{\varepsilon},$$

where $\vec{\varepsilon}$ is electrical field and $\vec{J}$ is electric current density. An expression of σ can be derived.

5.6 Mass diffusion
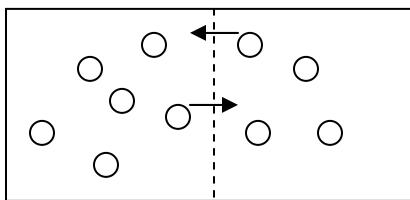
6. To understand transport and energy conversion, we need to know:
— How much energy/momentum can a particle have?
— How many particles have the specified energy E?
— How fast do they move?
— How far can they travel?
— How do they interact with each other?

6.1 How much energy/momentum can a particle have?

	Classical mechanics	Quantum mechanics
Energy	$E = E_{\text{Kinetic}} + E_{\text{Potential}}$	E is the eigenvalue of the Schrödinger equation
E_{Kinetic}	$E_{\text{Translation}} = \dfrac{mv^2}{2}$ (for quantum case, I did not give answer but point out it is the solution for particle in a box)	
	$E_{\text{Vibration}} = \dfrac{mv^2}{2} + \dfrac{Kx^2}{2}$	$E_{\text{Vibration}} = h\nu(n+\dfrac{1}{2}); \nu = \dfrac{1}{2\pi}\sqrt{\dfrac{K}{m}}$ (n=0,1,2$\cdots$)
	$E_{\text{Rotation}} = \dfrac{I\omega^2}{2}$	$E_{\text{Rotation}} = hBl(l+1)$ (l=0,1$\cdots$)

Here the Planck constant $h = 6.6 \times 10^{-34} J \cdot s$. The vibration energy of a standing wave inside the potential well is discrete in quantum mechanics. In the table, we give the allowed energy levels of a harmonic oscillator, which is a model for the vibrations of a diatomic molecule such as H_2. The dispersion relation (E-**k** relation) for electrons, phonons, and photons are sketched in following figures, in which the wavevector **k** points to the direction of wave propagation (electron, photon, and phonon waves).
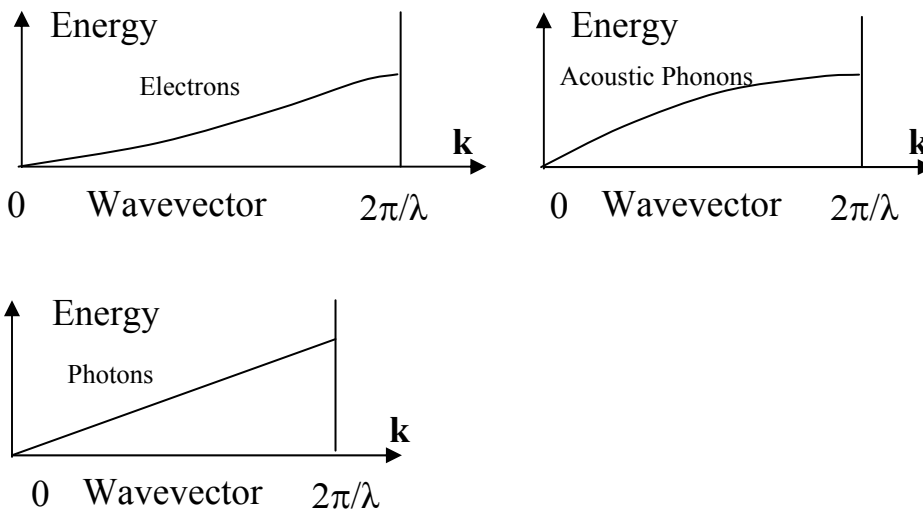
For photons, the energy is just a linear function of the wavevector, i.e.,

$$E = hc/\lambda = \frac{hc}{2\pi}\frac{2\pi}{\lambda} = \frac{hc}{2\pi}|\vec{k}|.$$

6.2 How many particles have the specified energy E?

For a monoatomic ideal gas system, the only energy of each atom is their kinetic energy,

$$E = \frac{m}{2}\left(v_x^2 + v_y^2 + v_z^2\right).$$

Statistical thermodynamics gives the probability density f(E), defined as the probability of finding the carriers at energy E per energy interval surrounding E, that a particle in an equilibrium system at a temperature T as,

$$f(E) = Ae^{-E/(\kappa_B T)},$$

where the Boltzmann constant k_B=1.38e-23 J/K.

6.3 How fast do they move?

First we use normalization of f to calculate A. Since the probability of finding this particle having energy between 0 and infinity must be one, we have

$$\int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} f(v_x,v_y,v_z)dv_z = 1.$$

Using spherical coordinates can simplify the calculation as

$$\int_0^{\infty} 4\pi v^2 f(v)dv = 1.$$

Both of above equations yield

$$A = \left(\frac{m}{2\pi k_B T}\right)^{3/2}.$$

Thus

$$f(\mathbf{v}) = \left(\frac{m}{2\pi\kappa_B T}\right)^{3/2} \exp\left[-\frac{m\left(v_x^2 + v_y^2 + v_z^2\right)}{2\kappa_B T}\right],$$

which is also called the Maxwell distribution. The average energy of the monoatomic gas is

$$\langle E \rangle = \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} \frac{m}{2}\left(v_x^2 + v_y^2 + v_z^2\right)\left(\frac{m}{2\pi\kappa_B T}\right)^{3/2} \exp\left[-\frac{m\left(v_x^2 + v_y^2 + v_z^2\right)}{2\kappa_B T}\right]dv_z$$

$$= \frac{3}{2}k_B T$$

At room temperature (300 K), this average energy is 39 meV, or 6.21e-21 J. For He gas, m=6.4e-27 kg. Using $\frac{mv^2}{2} = \frac{3}{2}k_B T$, we can calculate average v=1000 m/s, while it becomes 500 m/s for air. It is good to remember that $k_B T$ at room temperature is 26 meV.

Note: The flux of quantity X (e.g. momentum, energy) is expressed as $n(X)X \cdot v$, which is already used in 5.4.

6.4 How far can they travel?

The effective diameter for two atoms to collide is 2D. . If the number concentration is n [m⁻³], then the number of molecules that this particle will collide with is $n\pi D^2 L$. The average distance L between each collision satisfies $n\pi D^2 L = 1$.
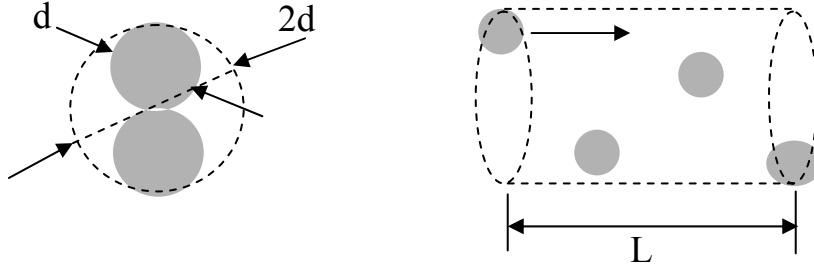
Thus the mean free path is

$$\Lambda = \frac{1}{n\pi D^2} \, .$$

Noticing $n = \rho / m$, where m is molecular weight, ρ is density. For ideal gases, we have $P = \rho RT$. Therefore,

$$\Lambda = \frac{m}{\pi D^2 \rho} = \frac{mRT}{\pi D^2 P} = \frac{R_u T}{\pi D^2 P N_A} = \frac{k_B T}{\pi D^2 P} \, ,$$

where the universal gas constant $R_u = N_A k_B = 8.314 J / mol \cdot K$.

The ideal gas law can also be derived as following:

In section 5.4, we derive $P = mn \frac{v^2}{3}$. In section 6.3, we get $\frac{mv^2}{2} = \frac{3}{2} k_B T$. Thus

$$P = mn \frac{v^2}{3} = nk_B T = \frac{N}{V} k_B T = \frac{N}{N_A} \frac{N_A}{V} k_B T = \frac{N}{N_A} \frac{R_u}{V} T \, , \text{ or } PV = \bar{N} R_u T \text{, in which } \bar{N} \text{ is}$$

the mole number.

At room temperature, atmosphere pressure, the mean free path is

$$\Lambda = \frac{k_B T}{\sqrt{2}\pi D^2 P} = \frac{1.38\text{e-}23 \times 300}{\sqrt{2}\pi \times (2.5\text{e-}10)^2 \times 1.01\text{e}5} = 0.14 \mu m \, ,$$

in which $\sqrt{2}$ comes when we consider relative velocity instead of assuming other particles are stationary. The collision time (relaxation time) is $\tau = \Lambda / \bar{v} \sim 10^{-10} s$.

For P=1 mTorr, we have $\Lambda = 0.1m$. The molecules seldom collide with each other.
Note: This relaxation time is not very small for current technology. For short-pulse lasers, the shortest period is only a few fs.

6.5 How do they interact with each other?

The collisions between particles can be elastic or inelastic. In a solar cell, the photon excites electrons to generate an output voltage. Energy conversion is closely associated with transport.
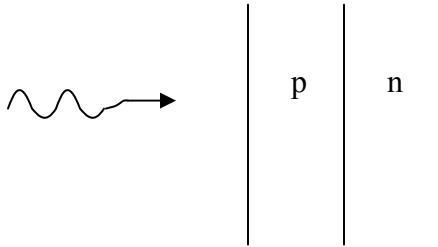
7. Simple kinetic theory

In the figure, half of the carriers within $v_x\tau$ can go across the interface before being scattered. Here v_x is the x component of the random velocity of the heat carriers and τ is the relaxation time — the average time a heat carrier travels before it is scattered and changes its direction. So the net heat flux carried by heat carriers across the interface is

$$q_x = \frac{1}{2}(nEv_x)\big|_{x-v_x\tau} - \frac{1}{2}(nEv_x)\big|_{x+v_x\tau} .$$
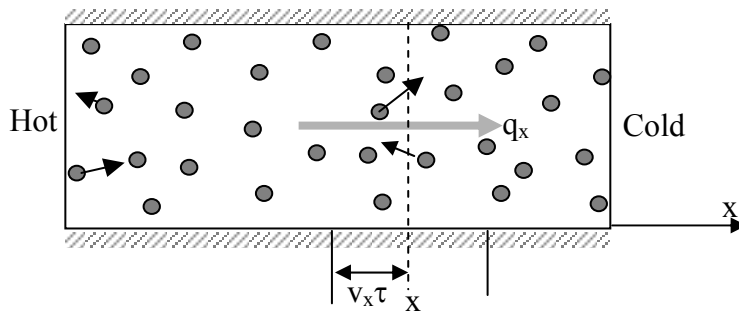
Using a Taylor expansion, we can write the above relation as

$$q_x = -v_x\tau\frac{d(nEv_x)}{dx}$$

$$= -v_x{}^2\tau\frac{d(nE)}{dx}$$

$$= -v_x{}^2\tau\frac{du}{dT}\frac{dT}{dx} .$$

Notice specific heat $C = du/dT$, $v_x{}^2 = v^2/3$. The above equation changes into

$$q_x = -\frac{v^2}{3}\tau C\frac{dT}{dx} .$$

Compared with the Fourier's law, we know that thermal conductivity $k = \dfrac{\tau C v^2}{3}$. The capital C is specific heat per unit volume, C=ρc.