4.1.1 Photons (continue)
First let us continue the discussion of photons. We have

$$\langle n \rangle = f(\omega, T) = \frac{1}{e^{\hbar\omega/k_B T} - 1}.$$

The internal energy is

$$u = \sum_{k_x}\sum_{k_y}\sum_{k_z} \hbar\omega f(\omega, T) = \int_0^\infty \hbar\omega f(\omega, T) D(\omega)d\omega,$$

where the density of states (two transverse electromagnetic waves) is

$$D(\omega) = 2 \times \frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3 d\omega} = \frac{\omega^2}{\pi^2 c^3}; \omega = ck \text{ for light.}$$

Thus

$$u = \int_0^\infty \hbar\omega \frac{\omega^2}{\pi^2 c^3} \frac{1}{\left[\exp\left(\hbar\omega/\kappa_B T\right) - 1\right]} d\omega = \int_0^\infty u_\omega d\omega,$$

in which we define

$$u_\omega = f(\omega, T)\hbar\omega D(\omega) = \frac{\hbar}{\pi^2 c^3} \frac{\omega^3}{\left[\exp\left(\hbar\omega/\kappa_B T\right) - 1\right]}.$$

Recall the Planck's law as

$$e_{b,\lambda} = \frac{c_1}{\lambda^5 (e^{c_2/\lambda T} - 1)},$$

which has λ^5 but in u_ω we have ω^3. Noticing $u_\lambda = \left|\frac{\Delta\omega}{\Delta\lambda}\right| u_\omega$ and $\omega = ck = 2\pi c/\lambda$, we

obtain $u_\lambda = \left|\frac{d\omega}{d\lambda}\right| u_\omega = \frac{2\pi c}{\lambda^2} u_\omega$, which accounts for the power difference in above two
expressions. Therefore, we have obtained the exact Planck's blackbody radiation law. The radiation intensity, defined as energy flux per unit solid angle and normal area, is calculated as

$$I_\lambda = \frac{cu_\lambda}{4\pi},$$

where 4π is the full solid angle (for sphere $\Omega = Area/R^2 = 4\pi$), c is light speed.
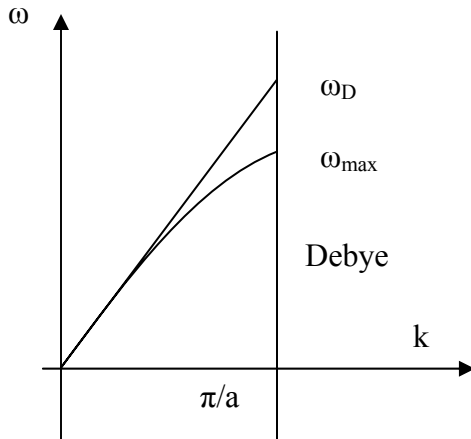
With $u = \int_0^\infty u(\omega)d\omega = \frac{4\sigma}{c}T^4$, the blackbody emissive power is expressed as

$e_b = \pi I = \sigma T^4$, where $\sigma = 5.67 \times 10^{-8} W/m^2 \cdot K^4$.

4.1.2 Phonons

In the Debye model, we assume $\omega = v_D |k|$. The maximum frequency is thus $\omega_D = v_D \dfrac{\pi}{a}$, which is different from original ω_{max}. For phonons, we have three polarizations (two transverse, one longitudinal waves). Similar to photons, we have

$$D(\omega) = \frac{dN}{Vd\omega} = 3 \bullet \frac{\omega^2}{2\pi^2 v_D^{\,3}} .$$

The internal energy is

$$U = \sum_{k_x}\sum_{k_y}\sum_{k_z} \hbar\omega f(T,\omega)$$

$$= \int_0^{\omega_D} \hbar\omega f(T,\omega) D(\omega) d\omega$$

$$= \frac{3}{2\pi^2 v_D^{\,3}} \int_0^{\omega_D} \frac{\hbar\omega^3 d\omega}{\exp(\hbar\omega/\kappa_B T) - 1} .$$

Note: For one monoatomic chain with N atoms, we have N quantum states. Similarly, for N atoms in a crystal, we have 3N quantum states (three acoustic branches) for phonons. This yields

$$3N/V = \frac{1}{V}\sum_{k_x}\sum_{k_y}\sum_{k_z} 1 = \int_0^{\omega_D} D(\omega)d\omega = \int_0^{\omega_D} \frac{3\omega^2}{2\pi^2 v_D^{\,3}} d\omega = \frac{\omega_D^{\,3}}{2\pi^2 v_D^{\,3}} ,$$

from which we can estimate ω_D and the effective lattice constant $a = v_D \dfrac{\pi}{\omega_D}$.

Define Debye temperature $\theta_D = \hbar\omega/k_B$. The specific heat is expressed as

$$C_V = 9k_B \frac{N}{V}\left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{x^4 e^x dx}{(e^x - 1)^2} ,$$

in which $x = \dfrac{\hbar\omega}{k_B T}$.

At low temperatures, the upper limit of above integration $\theta_D / T \to \infty$ and thus $C_V \propto T^3$, while in the high-temperature limit we have constant $C_V = 3\dfrac{N}{V} k_B$.

Note: At high temperatures, in each direction both the harmonic component $\dfrac{Kx^2}{2}$ and kinetic component $\dfrac{mv^2}{2}$ contribute $k_B T / 2$ to the internal energy. Vibrations of one ion in three directions totally contribute $k_B T$, which is consistent with $C_V = 3\dfrac{N}{V} k_B$. This result is similar to the ideal gas case. A common Cv-T curve is drawn as following.
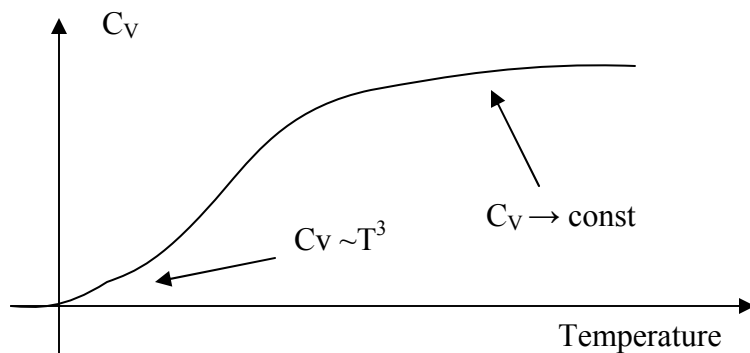
In many sources, people use the specific heat per unit mass instead of per unit volume. This normally causes a factor difference. In general, we have $Cv \sim 10^6 \; J/K \cdot m^3$.
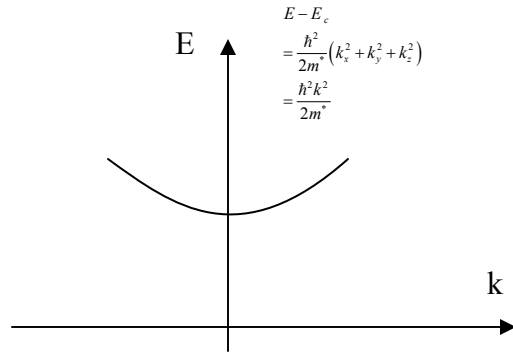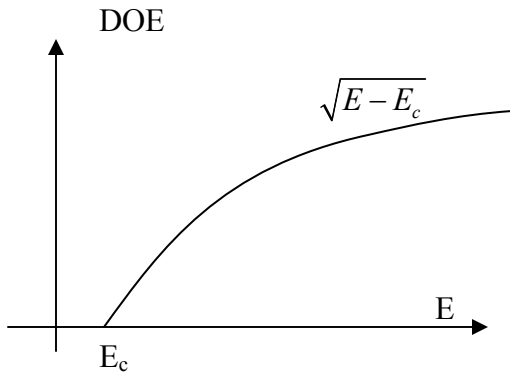
4.1.3 Electrons
In this case, the internal energy per unit volume is

$$U(T) = 2\sum_{k_x}\sum_{k_y}\sum_{k_z} Ef(E,T,\mu) = \int_{E_c}^{\infty} Ef(E,T,\mu)D(E)dE,$$

where the Fermi-Dirac distribution is $f = \dfrac{1}{e^{(E-\mu)/k_B T} + 1}$, the coefficient 2 for spins is included in D(E), the energy dispersion $E - E_c = \dfrac{\hbar^2}{2m^*}\left(k_x^2 + k_y^2 + k_z^2\right)$.

We can use the same idea as phonons to solve μ,

$$\frac{N}{V} = \frac{2}{V}\sum_{k_x}\sum_{k_y}\sum_{k_z} f(E,\mu,T)$$

$$= \frac{2}{V}\iiint_V f(E,\mu,T)\left(\frac{dk_x}{2\pi/L}\right)\left(\frac{dk_y}{2\pi/L}\right)\left(\frac{dk_z}{2\pi/L}\right)$$

$$= \int_0^\infty f(E,\mu,T)D(E)dE,$$

where N is the total number of electrons, and we use density of state to rewrite the summation in an integral form. The chemical potential μ is solved if N/V is given.

The specific heat is derived as

$$C_e = \frac{\partial u}{\partial T} = \frac{1}{2}\pi^2 \frac{N}{V}k_B\frac{T}{T_f},$$

in which the Fermi temperature is defined as $T_f = \dfrac{E_f}{k_B}$.

Note: (1) When we calculate $\sum_{k_x}\sum_{k_y}\sum_{k_z} f(E,\mu,T)$, the energy values within the energy gap should be excluded and we should not count the corresponding wavevectors. (2) In a semiconductor, the phonons contribute much more to the specific heat than electrons. Electron contribution can only exceed that of the phonon at very low temperatures in the following figure. In the equation $k = \dfrac{Cv\Lambda}{3}$, there are different specific heat C and velocity v for electrons and phonons. We should also have different mean free paths. (3) For nanostructures, the energy is quantized and the summation should be conducted over the quantum numbers instead of wavevectors, such as quantum dots. (4) All current discussions are based on equilibrium state. We will talk about nonequilibrium problems later.
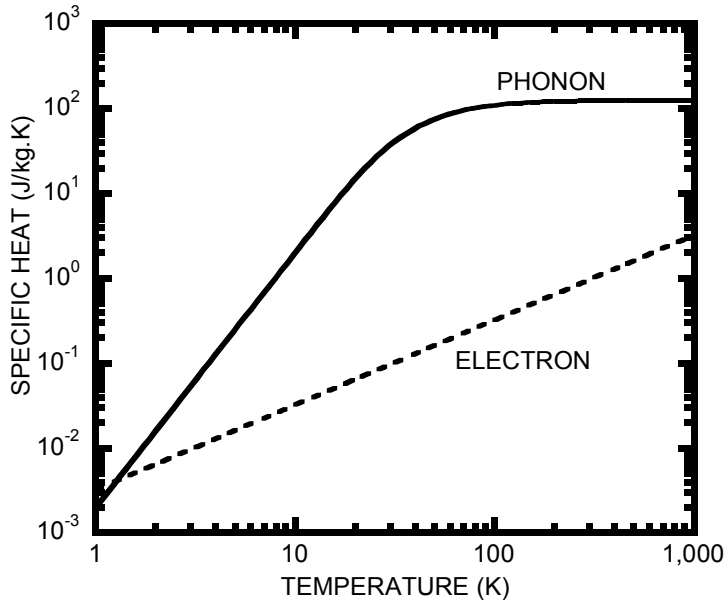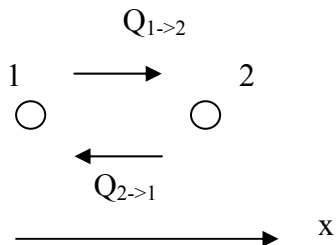
Chapter 5 Energy transport by waves

Consider energy transported between two points. The net energy transfer rate is

$$q_{12} = q_{1\to2} - q_{2\to1} = \int \tau_{1\to2} v_x E_1 f(T, E_1) D(E_1) dE_1,$$

in which $\tau_{1\to2}$ is the transmissivity, $E_1 f(T, E_1) D(E_1)$ has the unit J/m^3, and q_{12} has the unit W/m^2.

Now the question is how to calculate the transmissivity τ and velocity v. For nanostructures, the interface characteristic length is comparable to wavelength so that the interface is important even in the classic viewpoint.

5.1 Plane waves & their interface reflection
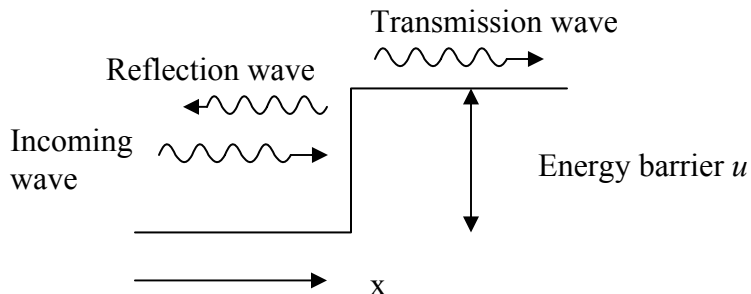
Recall the above homework problem. Generally we have the wavefunction of the transmitted wave as

$$\Psi_t(t,x) = e^{-i\frac{E}{\hbar}t}\Psi(x) = e^{-i(\omega t - k_x x)},$$

in which $k_x = \sqrt{\dfrac{2m(E-u)}{\hbar^2}}$.

Based on the Schrödinger equation

$$-\frac{\hbar}{2m}\nabla^2\Psi + (U-E)\Psi = 0,$$

we have

$$\Psi_i = Ae^{-i(\omega t - k_1 x)} \quad \text{(incoming wave)},$$

$$\Psi_r = Be^{-i(\omega t + k_1 x)} \quad \text{(reflected wave)}, \quad k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\Psi_t = Ce^{-i(\omega t - k_2 x)} \quad \text{(transmitted wave)}, \quad k_2 = \sqrt{\frac{2m(E-u)}{\hbar^2}} .$$

The boundary conditions are applied

$$(\Psi_i + \Psi_r)_{x=0^-} = \Psi_t\,|_{x=0^+}, \quad (\Psi_i' + \Psi_r')_{x=0^-} = \Psi_t'\,|_{x=0^+},$$

which yields

$$A + B = C; \quad k_1(A-B) = k_2 C$$

or $\dfrac{B}{A} = \dfrac{k_1 - k_2}{k_1 + k_2}; \dfrac{C}{A} = \dfrac{2k_1}{k_1 + k_2}$.

The flux term is (note A and k_1 can be complex)

$$J = \mathrm{Re}\left(\frac{i\hbar}{m}\Psi\nabla\Psi^*\right)$$

$$= \mathrm{Re}\left(\frac{i\hbar}{m}Ae^{-i(\omega t - k_1 x)}A^*(-ik_1^*)e^{i(\omega t - k_1^* x)}\,|_{x=0}\right)$$

$$= \frac{\hbar}{m}|A|^2\,\mathrm{Re}\left(k_1^*e^{i(k_1 - k_1^*)x}\,|_{x=0}\right)$$

$$= \frac{\hbar}{m}|A|^2 k_1,$$

where we use the fact that k_1 is a real number in the last step.