Exercise 4.1

Electrons in semiconductors. A semiconductor has a parabolic band structure:

$$E - E_c = \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2 + k_z^2)$$

The Fermi level in the semiconductor could be above or below the conduction band edge. Take the electron effective mass as the free electron mass. For $\mu - E_c = 0.05eV$ and $T = 300K$, do the following in the range $0.0eV < E - E_c < 0.1eV$:

a) Plot the Fermi-Dirac distribution as a function of E.

b) Plot the density of state as a function of E.

c) Calculate the product of $f(E,T)D(E)$, which means the average number of eletrons at each E, and plot the product as a function of E.

d) Calculate the product of $(E - E_c)f(E,T)D(E)$, which means the actual kinetic energy at each allowable energy level, and plot the product as a function of E.

e) Repeat the questions for $\mu - E_c = -0.05eV$.

Solution

a) We can rewrite the Fermi-Dirac distribution based on the relative Fermi level position($\mu - E_c = 0.05eV$) with respect to conduction band edge E_c:

$$f(E,T) = f(E,300K) = 1/(e^{\frac{(E-(0.05+E_c)}{8.617\cdot10^{-5}\cdot300}} + 1)$$

Plotting $f(E,T)$ in the range $0 < E - E_c < 0.1eV$, we get :

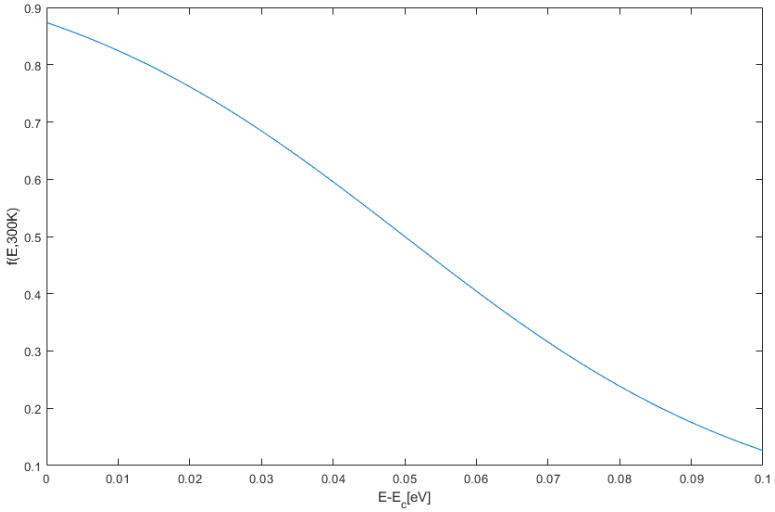


Figure 1: Fermi-Dirac distribution as a function of $E - E_c$

b) Density of state of spherical parabolic band per unit volume and per unit energy interval can be written as (See lecture 5, slide 37 for the derivation) :

$$D(E) = \frac{1}{2\pi^2}(\frac{2m^*}{\hbar^2})^{\frac{3}{2}}(E - E_c)^{\frac{1}{2}}$$

Considering free electron mass, $m^* = 9.1\times10^{-31}kg$ and the unit conversion $1kg = 6.24\cdot10^{18}eV\cdot m^{-2}\cdot s^2$, plotting the $D(E)$ in the range $0 < E - E_c < 0.1eV$, we get :

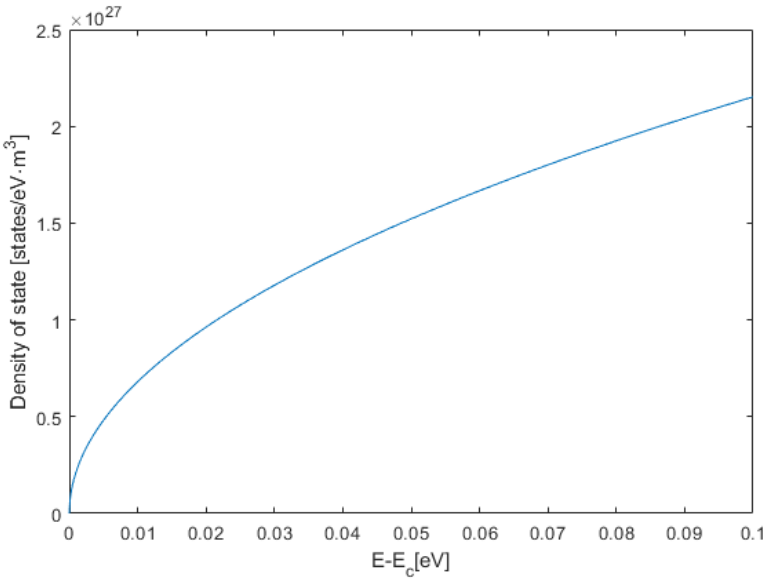


Figure 2: Electron density of state as a function of $E - E_c$

c) Plot of $f(E, 300K)D(E)$ in the range gives :

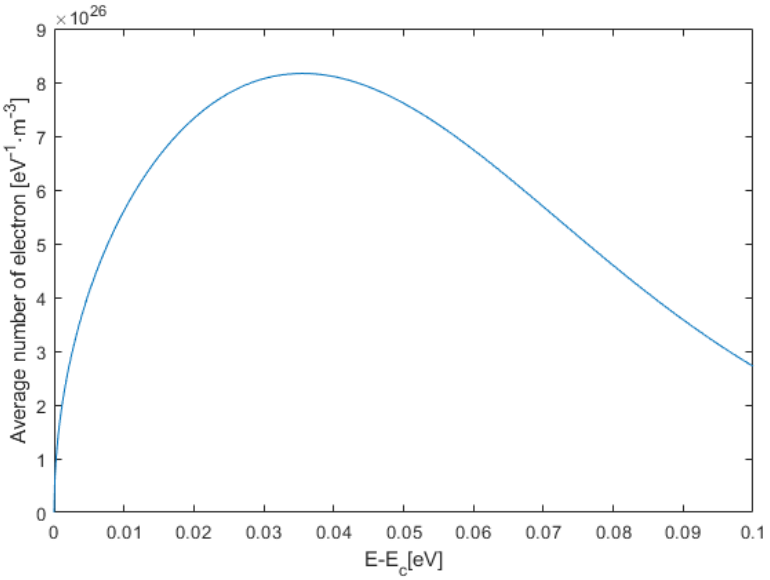


Figure 3: Average number of electrons as a function of $E - E_c$

d) Plot of $(E - E_c)f(E, 300K)D(E)$ in the range gives :

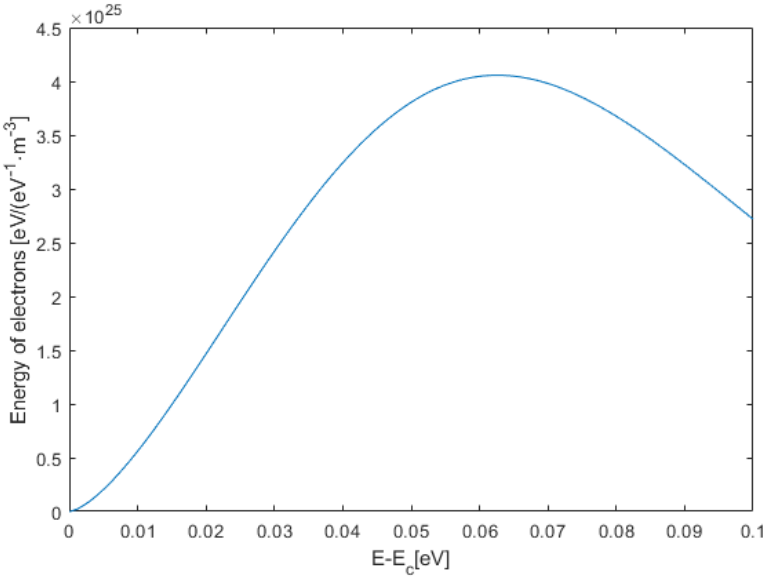


Figure 4: Kinetic energy of electrons as a function of $E - E_c$

e) Now, Fermi energy level lies 0.05eV below the conduction band edge E_c. Shift in Fermi energy basically shifts overall the Fermi-Dirac distribution. Therefore, we expect change in $f(E,T)D(E)$, $(E-E_c)f(E,T)D(E)$ energy distribution as well but not the density of state of electron, which remains the same regardless of the Fermi level position. Fermi-Dirac distribution when the Fermi energy level lies 0.05eV below the conduction band edge E_c is written as:

$$f(E,T) = f(E,300K) = 1/(e^{\frac{(E-(-0.05+E_c)}{8.617\cdot10^{-5}\cdot300}} + 1)$$

Plotting this distribution in the same energy range, we get:

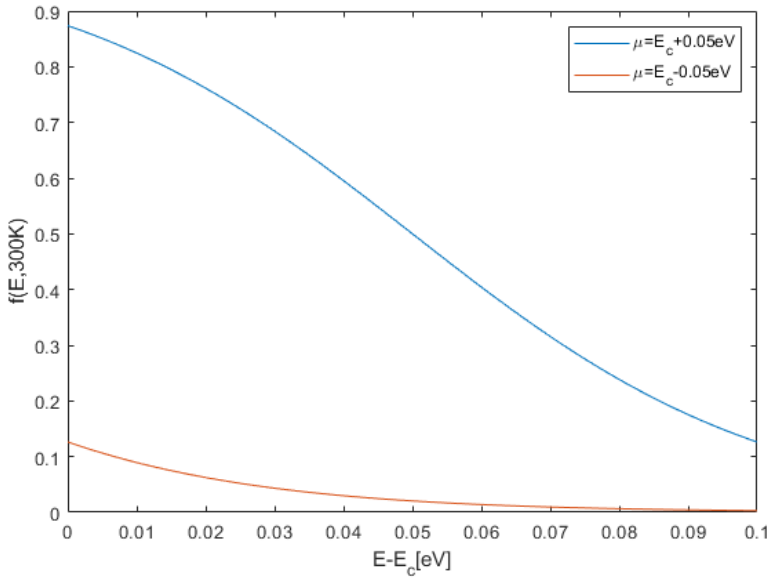


Figure 5: Fermi-Dirac distribution as a function of $E-E_c$. Blue(orange) line corresponds to Fermi level above(below) the conduction band edge.

Orange line in the above figure refers to the Fermi-Dirac distribution at $\mu - E_c = -0.05eV$.

Plotting similarly $f(E,300K)D(E)$ and $(E-E_c)f(E,300K)D(E)$ when $\mu - E_c = -0.05eV$ gives:

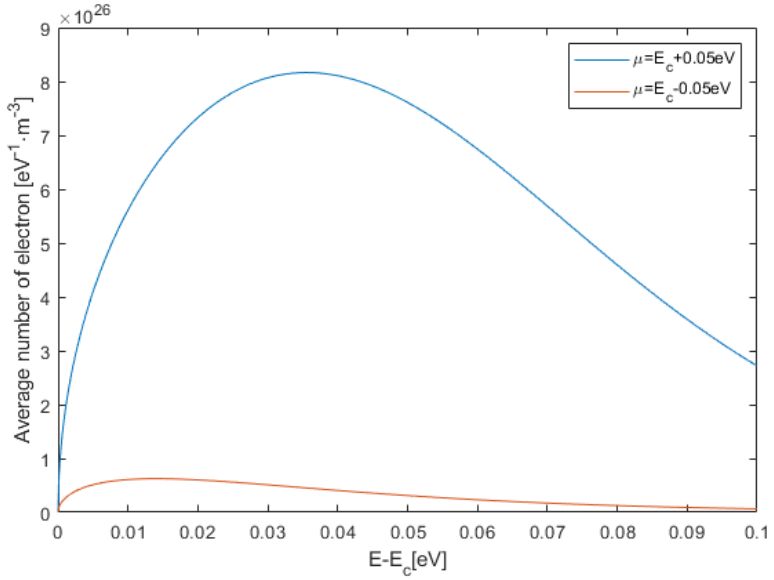


Figure 6: Average number of electrons as a function of $E-E_c$. Blue(orange) line corresponds to Fermi level above(below) the conduction band edge.

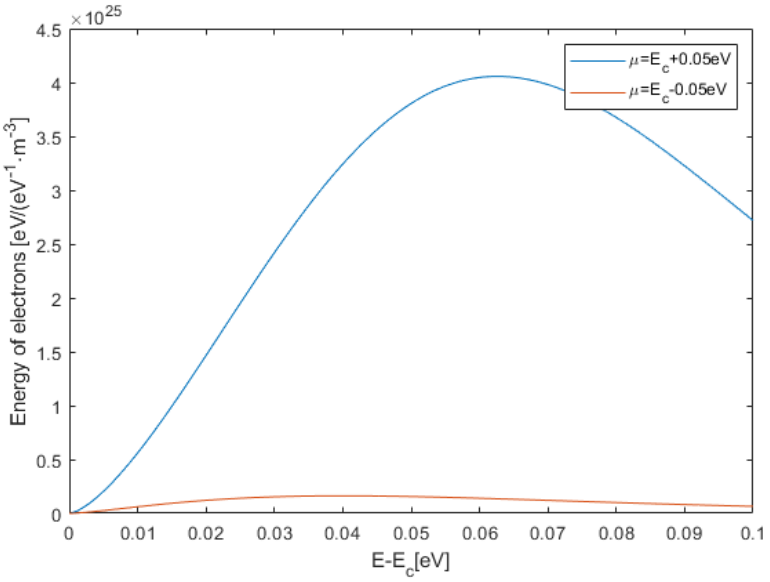


Figure 7: Kinetic energy of electrons as a function of $E - E_c$. Blue(orange) line corresponds to Fermi level above(below) the conduction band edge.

As Fermi level moves away from the edge of conduction band toward the bandgap, lesser number of electron will be excited in the conduction band at 300K.

Exercise 4.2

Chemical potential and dopant concentration. The number of electrons in the conduction band can be assumed to be equal to the dopant concentration. Calculate the chemical potential levels relative to the band edge for the dopant concentrations of 10^{18} cm^{-3} and 10^{19} cm^{-3}.
Assume the effective electron mass is approximated to free electron mass at $T = 300K$.
It is given that the density of states for electron is $D(E)$, where

$$D(E) = \frac{1}{2\pi^2}\left[\frac{2m^*}{\hbar^2}\right]^{3/2}(E - E_c)^{1/2}$$

and , E_c is the energy of the conduction band edge.

Solution

In order to obtain the number of all available states, we can integrate the density of states for all possible values of Energy. However, to obtain the number of occupied states we need to include the probability of an states being occupied which is given by Fermi-Dirac distribution, which is a function of energy level, chemical potential and temperature.

$$f(E,\mu,T) = \frac{1}{e^{\frac{E-\mu}{k_B T}} + 1}$$

If n is the number of occupied states, then n is can be expressed as:

$$n = \int_{E_c}^{\infty} f(E,\mu,T) D(E)\, dE$$

$$n = \int_{E_c}^{\infty} \frac{1}{e^{\frac{E-\mu}{k_B T}} + 1} \frac{1}{2\pi^2} \left[\frac{2m^*}{\hbar^2}\right]^{3/2} (E - E_c)^{1/2}\, dE$$

$$n = \frac{1}{2\pi^2} \left[\frac{2m^*}{\hbar^2}\right]^{3/2} \int_{E_c}^{\infty} \frac{1}{e^{\frac{E-\mu}{k_B T}} + 1} (E - E_c)^{1/2}\, dE$$

The above integral can be evaluated numerically and is a function of chemical potential and temperature. Therefore, one can obtain the value of chemical potential for specified values of dopant concentration and temperature. However, if we make a classical assumption, the integral can be solved analytically. This holds good at lower temperature, when $\frac{E-\mu}{k_B T} >> 1$ and as a result Fermi-Dirac distribution is approximated to Boltzmann distribution.

$$e^{\frac{E-\mu}{k_B T}} + 1 \approx e^{\frac{E-\mu}{k_B T}}$$

$$n = \frac{1}{2\pi^2} \left[\frac{2m^*}{\hbar^2}\right]^{3/2} \int_{E_c}^{\infty} e^{-\frac{E-\mu}{k_B T}} (E - E_c)^{1/2}\, dE$$

substituting $z = \frac{E-E_c}{k_B T}$ in the above integral, we get,

$$n = \frac{1}{2\pi^2} \left[\frac{2m^* k_B T}{\hbar^2}\right]^{3/2} e^{-\frac{E_c-\mu}{k_B T}} \int_0^{\infty} e^{-z} z^{1/2}\, dz$$

$$n = \frac{1}{2\pi^2} \left[\frac{2m^* k_B T}{\hbar^2}\right]^{3/2} e^{-\frac{E_c-\mu}{k_B T}} \times \frac{\sqrt{\pi}}{2}$$

$$n = 2 \left[\frac{2\pi m^* k_B T}{h^2}\right]^{3/2} e^{-\frac{E_c-\mu}{k_B T}}$$

Let,

$$N_c = 2 \left[\frac{2\pi m^* k_B T}{h^2}\right]^{3/2}$$

then,

$$E_c - \mu = k_B T \ln \frac{N_c}{n}$$

At $300K$,

$$N_c = 2 \times \left[\frac{2\pi \times 9.1 \times 10^{-31} \times 1.38 \times 10^{-23} \times 300}{(6.626 \times 10^{-34})^2}\right]^{3/2} = 2.5038 \times 10^{25} m^{-3} = 2.5038 \times 10^{19} cm^{-3}$$

a) $n = 10^{18}\ cm^{-3}$

$$E_c - \mu = 3.22 k_B T\ = 83.4\ meV$$

b) $n = 10^{19}\ cm^{-3}$

$$E_c - \mu = 0.918 k_B T\ = 23.77\ meV$$

Exercise 4.3

Blackbody radiation. Consider the Blackbody radiation at 300K.

a) Plot the Bose-Einstein distribution as a function of angular frequency ω

b) Plot the density of states as a function of ω

c) Plot fD as a function of ω

d) Plot $\hbar\omega fD$ as a function of ω

e) compute the emissive power as a function of temperature and the corresponding specific heat

f) Compare (a)-(e) for Photons and Phonons. Use Debye model with Debye velocity of 5000 m/s and Debye temperature 500 K

Solution

The Bose-Einstein distribution for bosons such as Photon, Phonon are expressed as:

$$f(\omega, T) = \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$

The density of states for photon and phonon(under Debye approximation) are expressed as below:

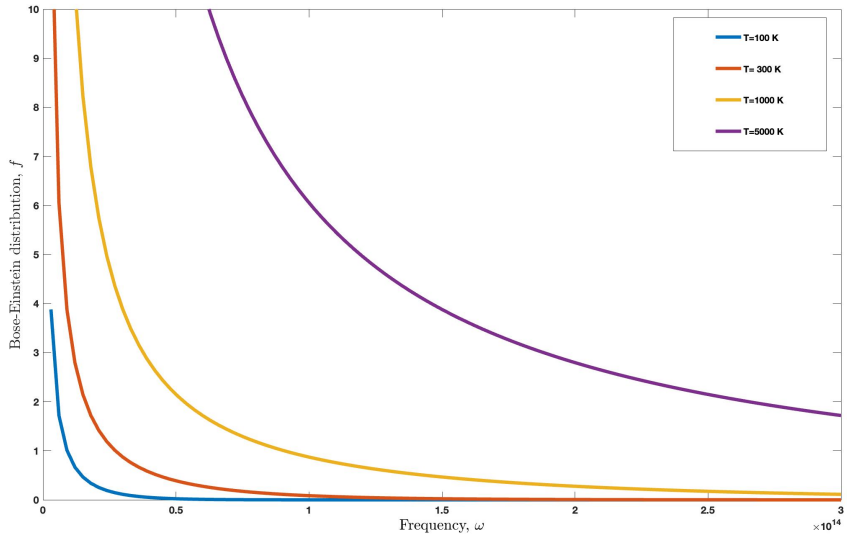


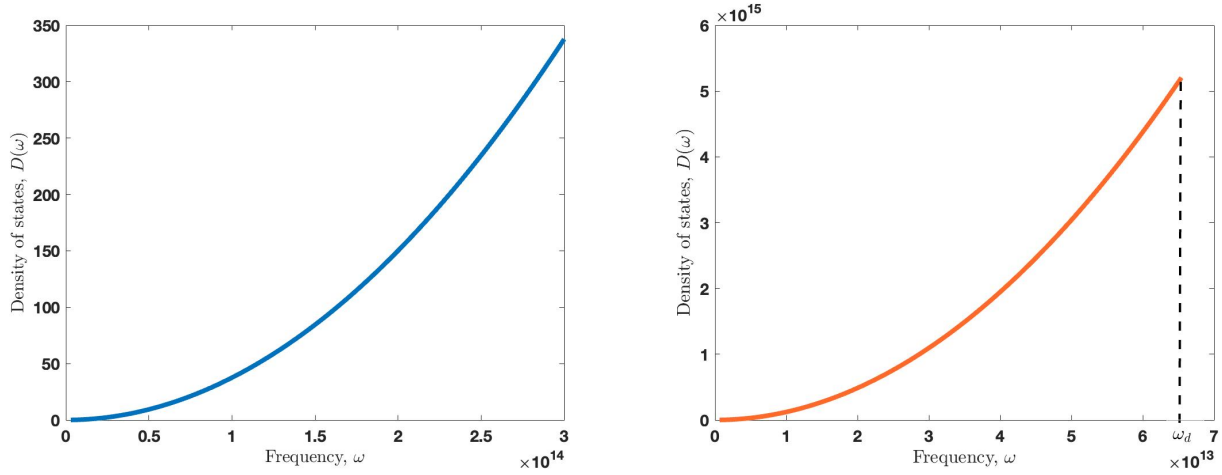
Figure 8: Bose-Einstein distribution as a function of frequency, $\omega$for various values of temperature

For photon,

$$D(\omega) = \frac{\omega^2}{\pi^2 c^3} \; for \; 0 < \omega < \infty$$

For photon,

$$D(\omega) = \frac{3\omega^2}{2\pi^2 {v_d}^3} \; for \; 0 < \omega < \omega_d$$

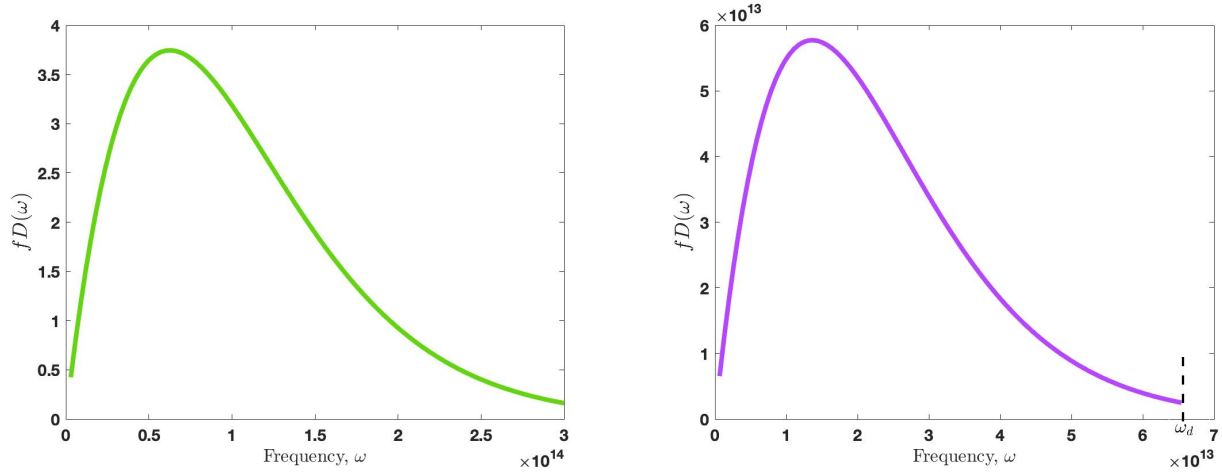


(a) Photon (b) Phonon, Debye approximation

Figure 9: Density of states for photon and phonon

Density of states gives the number of possible states (including the polarisation), and f is the average number of particles in each states.therefore, $fD(\omega)$ gives the average number of particles present in

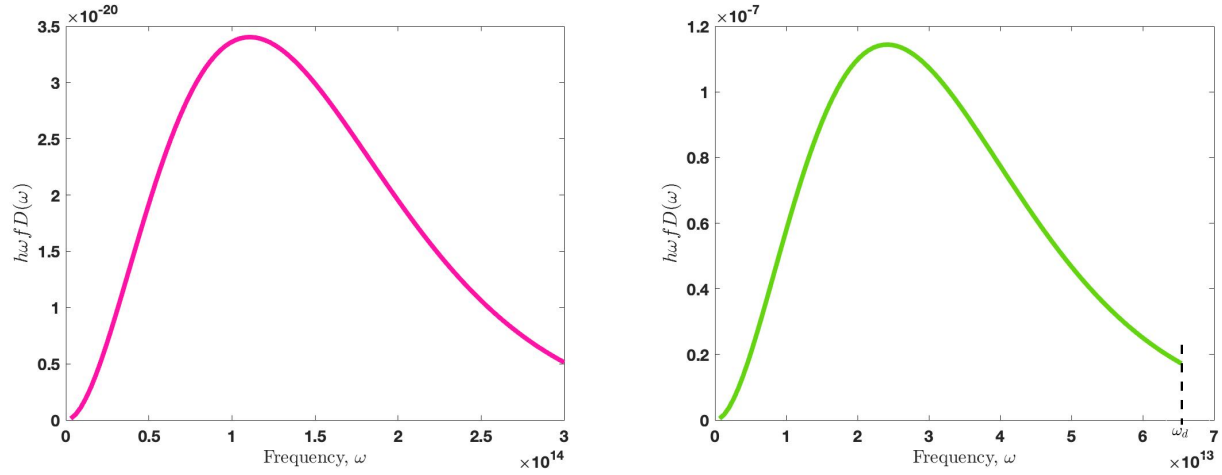
the given states.
Note that, the aggregation of particles in the same state, is a characteristic of particles obeying Bose–Einstein statistics.



(a) Photon (b) Phonon, Debye approximation

Figure 10: Density of number of particles for photon and phonon

The energy of each particles (photon or phonon) is $\hbar\omega$, therefore, $\hbar\omega f D(\omega)$ gives the energy density for an interval of frequency $d\omega$. The total energy density can be obtained by integrating it for all possible values of frequency. The total energy density for photon and phonon can be determined by



(a) Photon (b) Phonon, Debye approximation

Figure 11: Energy density for a frequency interval $d\omega$ for photon and phonon

the following expression:
for photon,

$$u = \frac{\hbar}{\pi^2 c^3} \int_0^\infty \frac{\omega^3}{e^{\frac{\hbar\omega}{k_B T}} - 1} d\omega$$

for phonon,

$$u = \frac{3\hbar}{2\pi^2 {v_d}^3} \int_0^{\omega_d} \frac{\omega^3}{e^{\frac{\hbar\omega}{k_B T}} - 1} d\omega$$

For photon, the intergral can be evaluated analytically, by use of proper substituion, $x = \frac{\hbar\omega}{k_B T}$

$$u = A_0 T^4 \int_0^\infty \frac{x^3}{e^x - 1} dx = A_1 T^4$$

where,

$$A_0 = \frac{\hbar}{\pi^2 c^3}\left(\frac{k_B}{\hbar}\right)^4$$

Since a photon propagates in all direction with speed c, the intensity is expressed as:

$$I = \frac{cu}{4\pi} = \frac{cA_1}{4\pi}T^4$$

where, the factor 4π is attributed to the total solid angle.
The emissive power is given by:

$$e = \pi I = \frac{cA_1}{4}T^4$$

The specific heat of a blackbody is proportional to T^3, which is expressed as:

$$specific\ heat = \frac{du}{dT} = 4A_1T^3$$

Note: Although, specific heat for phonon cannot be evaluated analytically, it is interesting to note that the specific heat behaviour of phonon at low temperature. It is indeed proportional to T^3, which is same as photon.

Exercise 4.4

Phonon specific heat Assuming that phonons obey the following dispersion relation (three-dimensional isotropic medium)

$$\omega = 2\sqrt{\frac{K}{m}}|sin\frac{|\mathbf{k}|a}{2}|$$

where a is the lattice constant, K the spring constant, and $\mathbf{k}$ the wavevector. Derive an expression for the phonon internal energy and specific heat.

Solution

Such dispersion relation corresponds to acoustic phonon mode. Although the acoustic phonon dispersion relation is non-linear, very often the Debye approximation ($\omega = \nu k$) is used, which assumes a linear dispersion relation between the frequency and the wavevector. It is especially a good approximation at low frequency range. We start with the approximation that

$$\omega = 2\sqrt{\frac{K}{m}}|sin\frac{|\mathbf{k}|a}{2}|= \sqrt{\frac{K}{m}}a|\mathbf{k}|= \nu|\mathbf{k}|$$

where ν is velocity of the sound wave.

Here, we assume that the medium holds only acoustic phonon mode, not the optical one (a case with 1 atom per lattice). From the lecture slide p.28, we know the phonon density of state can be written as

$$D(\omega) = \frac{k^2 V}{2\pi^2}\frac{d|k|}{d\omega}$$

Substituting with $|\mathbf{k}|= \frac{\omega}{\nu}$ and considering 3 polarizations of acoustic mode, we can rewrite it as

$$D(\omega) = \frac{3\omega^2 V}{2\pi^2\nu^3}$$

The phonon internal energy as a function of temperature can be calculated integrating all the possible phonon vibration frequencies upto cut off frequency(ω_D), which can be written as,

$$U = \int_0^{\omega_D} d\omega D(\omega)\hbar\omega\frac{1}{e^{\frac{\hbar\omega}{k_B T}}-1}$$

where ω_D, D(ω), $\hbar\omega$ and $\frac{1}{e^{\frac{\hbar\omega}{k_B T}}-1}$ are phonon cutoff frequency, phonon density of states, phonon energy at given frequency, and Bose–Einstein distribution, respectively.

Plugging above $D(\omega)$, we get phonon internal energy :

$$U = \int_0^{\omega_D} d\omega\frac{3\omega^2 V}{2\pi^2\nu^3}\hbar\omega\frac{1}{e^{\frac{\hbar\omega}{k_B T}}-1}$$

$$= \frac{3V\hbar}{2\pi^2\nu^3}\int_0^{\omega_D} d\omega\frac{\omega^3}{e^{\frac{\hbar\omega}{k_B T}}-1}$$

Phonon specific heat is calculated by differentiating the U with respect to temperature, T :

$$C = \frac{\partial U}{\partial T} = \frac{\partial}{\partial T}\left(\frac{3V\hbar}{2\pi^2\nu^3}\int_0^{\omega_D} d\omega\frac{\omega^3}{e^{\frac{\hbar\omega}{k_B T}}-1}\right)$$

$$= \frac{3V\hbar}{2\pi^2\nu^3}\frac{\hbar}{k_B T^2}\int_0^{\omega_D} d\omega\frac{\omega^4 e^{\frac{\hbar\omega}{k_B T}}}{(e^{\frac{\hbar\omega}{k_B T}}-1)^2}$$

If there are N lattices in the medium, there are 3N acoustic phonon modes. With this information, cut off frequency ω_D can be defined and be replaced in above equations with :

$$3N = \frac{3K^3 V}{6\pi^2} = \frac{3\omega_D^3 V}{6\pi^2\nu^3}$$

$$\omega_D = (\frac{6\pi^2\nu^3 N}{V})^{\frac{1}{3}}$$

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