

Thermal Energy at the Nanoscale

Homework Solution - Week 2

Spring 2013

1. Getting a feel for the numbers

(a) The Bose-Einstein distribution is given by:

$$f_{BE}^o = \frac{1}{\exp(E/k_B T) - 1} \quad (1)$$

At $T = 300$ K, $k_B T = 0.026$ eV. Thus, $f_{BE}^o = 0.002$ for $E = 0.16$ eV and $f_{BE}^o = 0.0003$ for $E = 0.21$ eV. At $T = 3000$ K, $k_B T = 0.258$ eV. Thus, $f_{BE}^o = 1.164$ for $E = 0.16$ eV and $f_{BE}^o = 0.796$ for $E = 0.21$ eV. The occupation numbers increase with increase in temperature (see Figure 1a). Also note that f_{BE}^o can be greater than 1 since the Pauli exclusion principle does not apply for bosons.

(b) The Fermi-Dirac distribution is given by:

$$f_{FD}^o = \frac{1}{\exp((E - \mu)/k_B T) + 1} \quad (2)$$

At $T = 1$ K, $k_B T = 8.63 \times 10^{-5}$ eV. Thus $f_{FD}^o = 1$ for $E = 1$ eV, $f_{FD}^o = 1$ for $E = 11.5$ eV and $f_{FD}^o = 0$ for $E = 20$ eV.

At $T = 3000$ K, $k_B T = 0.258$ eV. Thus $f_{FD}^o = 1$ for $E = 1$ eV, $f_{FD}^o = 0.68$ for $E = 11.5$ eV and $f_{FD}^o = 0$ for $E = 20$ eV. The Fermi-Dirac distribution changes from 1 to 0 in a small energy window (of the order of $k_B T$) around the electrochemical potential (see Figure 1b).

(c) From the given expression, the average thermal speed of argon atoms ($m = 40$ amu. = 6.64×10^{-26} kg) at $T = 300$ K is 398.8 m/s. Thus the average kinetic energy is:

$$E = \frac{1}{2} m_{Ar} v^2 = 0.033 \text{ eV} \quad (3)$$

The Maxwell-Boltzmann distribution is given by $f_{MB}^o = \exp(-E/k_B T) = 0.28$.

(d) For a given wavelength λ , the energy of the photon is given by $E = hc/\lambda$. Thus $E = 12.42$ eV for $\lambda = 100$ nm, $E = 2.07$ eV for $\lambda = 600$ nm and $E = 1.38$ eV for $\lambda = 900$ nm. Also $k_B T = 0.49$ eV at $T = 5700$ K. Thus $f_{BE}^o = 9.82 \times 10^{-12}$ for $\lambda = 100$ nm, $f_{BE}^o = 0.0148$ for $\lambda = 600$ nm and $f_{BE}^o = 0.063$ for $\lambda = 900$ nm.

2. Working with the Bose-Einstein distribution function

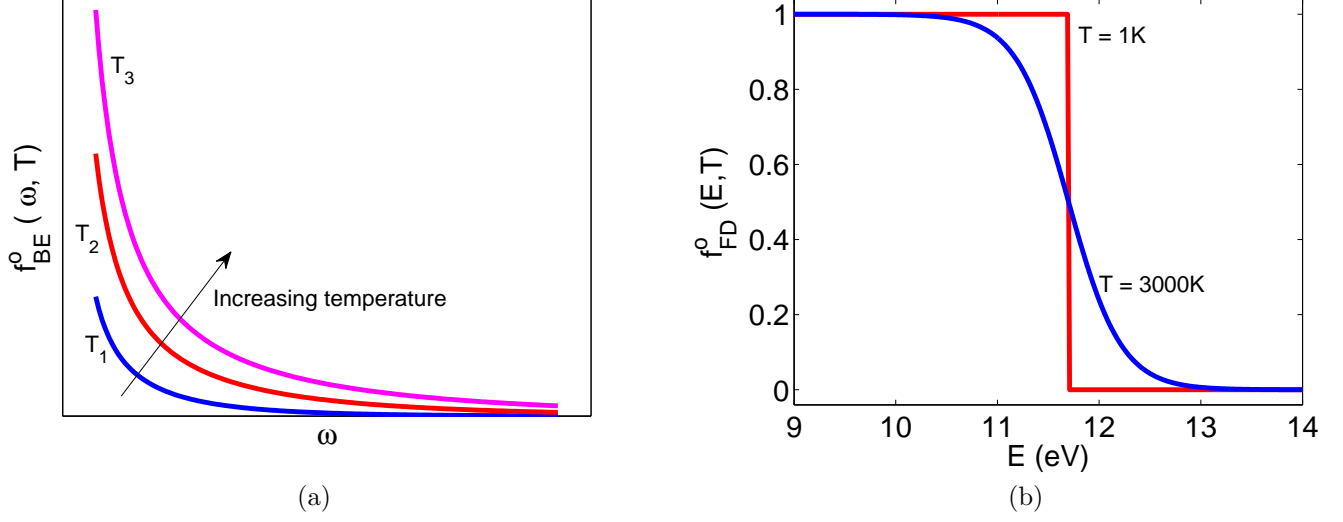


Figure 1: a) Bose-Einstein distribution function. b) Fermi-Dirac distribution function.

(a) The partition function Ξ is given by:

$$\begin{aligned}
 \Xi &= \sum_n \exp(-\beta E_n) \\
 &= \sum_{n=0}^{n=\infty} \exp(-\beta (n + 1/2) \hbar \omega) \\
 &= \frac{\exp(-\beta \hbar \omega / 2)}{1 - \exp(-\beta \hbar \omega)}
 \end{aligned} \tag{4}$$

(b) The average energy $\langle E \rangle$ is given by:

$$\begin{aligned}
 \langle E \rangle &= -\frac{\partial \ln \Xi}{\partial \beta} \\
 &= -\frac{\partial}{\partial \beta} \left(-\frac{\beta \hbar \omega}{2} - \ln(1 - \exp(-\beta \hbar \omega)) \right) \\
 &= \frac{\hbar \omega}{2} + \frac{\hbar \omega \exp(-\beta \hbar \omega)}{1 - \exp(-\beta \hbar \omega)} \\
 &= \hbar \omega \left(\frac{1}{\exp(\beta \hbar \omega) - 1} + \frac{1}{2} \right) \\
 &= \hbar \omega \left(f_{BE}^o + \frac{1}{2} \right)
 \end{aligned} \tag{5}$$

3. Phonon DOS in graphene

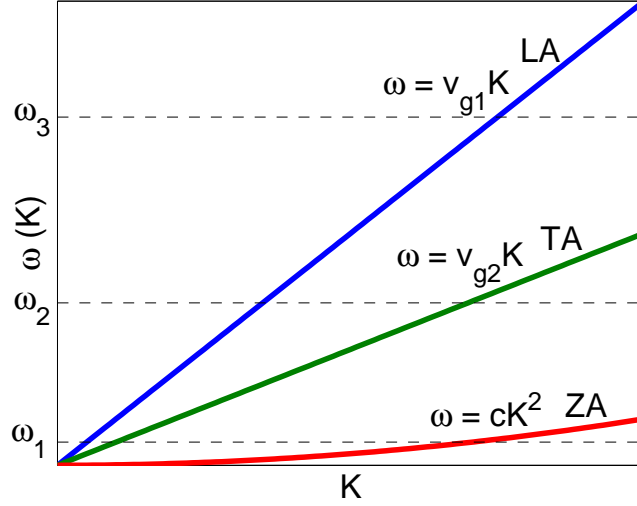


Figure 2: Graphene dispersion relation.

The DOS for the LA mode is given by:

$$\begin{aligned}
 D_{LA}(\omega) &= \frac{1}{L^2} \frac{dN}{dK} \frac{dK}{d\omega} \\
 &= \frac{1}{v_{g1} L^2} \frac{L^2 K}{2\pi} \left(N = \frac{\pi K^2}{(2\pi/L)^2}, \frac{d\omega}{dK} = v_{g1} \right) \\
 &= \frac{\omega}{2\pi v_{g1}^2}
 \end{aligned} \tag{6}$$

Similarly, the DOS for the linear TA mode is given by:

$$D_{TA}(\omega) = \frac{\omega}{2\pi v_{g2}^2} \tag{7}$$

The DOS for the quadratic ZA mode is given by:

$$\begin{aligned}
 D_{ZA}(\omega) &= \frac{1}{L^2} \frac{dN}{dK} \frac{dK}{d\omega} \\
 &= \frac{1}{2cK L^2} \frac{L^2 K}{2\pi} \left(N = \frac{\pi K^2}{(2\pi/L)^2}, \frac{d\omega}{dK} = 2cK \right) \\
 &= \frac{1}{4\pi c}
 \end{aligned} \tag{8}$$

All three modes are present at ω_1 . Thus,

$$\begin{aligned}
 D_{tot}(\omega_1) &= D_{LA}(\omega_1) + D_{TA}(\omega_1) + D_{ZA}(\omega_1) \\
 &= \frac{\omega_1}{2\pi v_{g1}^2} + \frac{\omega_1}{2\pi v_{g2}^2} + \frac{1}{4\pi c}
 \end{aligned} \tag{9}$$

Only the LA and TA modes are active at ω_2 :

$$\begin{aligned}
 D_{tot}(\omega_2) &= D_{LA}(\omega_2) + D_{TA}(\omega_2) \\
 &= \frac{\omega_2}{2\pi v_{g1}^2} + \frac{\omega_2}{2\pi v_{g2}^2}
 \end{aligned} \tag{10}$$

Only the LA mode is active at ω_3 :

$$\begin{aligned} D_{tot}(\omega_3) &= D_{LA}(\omega_3) \\ &= \frac{\omega_3}{2\pi v_{g1}^2} \end{aligned} \quad (11)$$

4. Wien's displacement law for phonons

Under the Debye approximation, the density of states $D(\omega)$ is given by:

$$D(\omega) = \frac{\omega^2}{2\pi^2 v_g^3} \quad (12)$$

The spectral energy density $u(\omega, T)$ is then given by:

$$\begin{aligned} u(\omega, T) &= \underbrace{\hbar\omega}_{\text{energy}} \underbrace{\frac{\omega^2}{2\pi^2 v_g^3}}_{\text{DOS}} \underbrace{\frac{1}{\exp(\hbar\omega/k_B T) - 1}}_{\text{occupation}} \\ &= \frac{\hbar}{2\pi^2 v_g^3} \frac{\omega^3}{\exp(\hbar\omega/k_B T) - 1} \end{aligned} \quad (13)$$

At a given temperature, spectral energy density is a maximum when $\frac{\partial u}{\partial \omega} = 0$. Thus,

$$3\omega^2(\exp(\hbar\omega/k_B T) - 1) - \omega^3 \exp(\hbar\omega/k_B T) \frac{\hbar}{k_B T} = 0 \quad (14)$$

Defining $x^* = \hbar\omega/k_B T$, we arrive at the following implicit equation for x^* .

$$3(1 - \exp(-x^*)) = x^* \quad (15)$$

The above equation can be solved numerically (using WolframAlpha for example) to obtain $x^* = 2.82$. Thus $\hbar\omega_{max} = 2.82k_B T$. The frequency at which the spectral energy distribution is a maximum increases linearly with temperature. In other words, the peak wavelength is inversely proportional to temperature. Figure 3 shows snapshots from the online CDF tool where the spectral energy distribution is plotted for three different temperatures. The peak of the curves moves to the right for increasing temperature. Use the online tool to tabulate ω_{max} for a few different temperatures and confirm the linear relationship between ω_{max} and T .

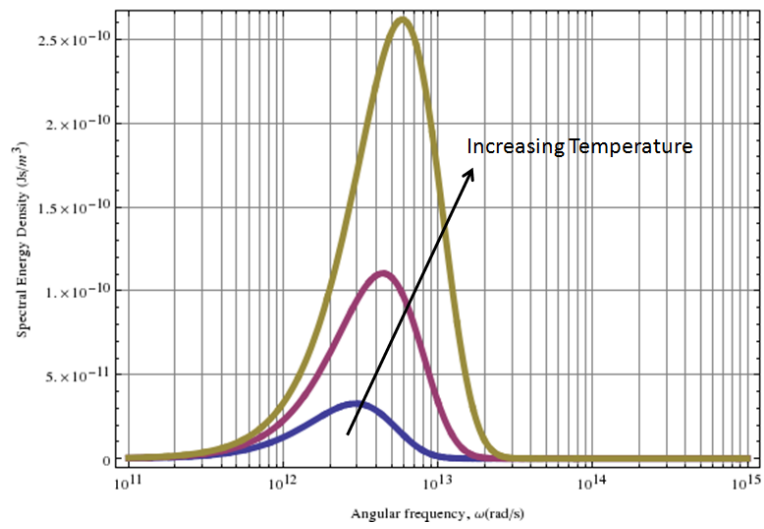


Figure 3: Spectral energy distribution for three different temperatures