8.08 Statistical Physics II

Phonons

(Dated: March 17, 2011)

1. Use the Debye approximation to find the following thermodynamic functions of a solid as a function of T.
   (a) $ln(Z)$
   (b) The mean energy
   (c) The entropy

   Express your answers in terms of the function $D(y) = \frac{3}{y^3}\int_0^y \frac{x^3 dx}{e^x - 1}$

   Solution:

   (a)

$$lnZ = \beta N\eta - \int_0^\infty ln(1 - e^{-\beta\hbar\omega})\sigma_D(\omega)d\omega$$

   where $\sigma_D(\omega) = \frac{3V}{2\pi^2 c^3}\omega^2$ for $\omega < \omega_D$ and 0 for $\omega > \omega_D$. Since $V = 6\pi^2 N(c/\omega_D)^3$ we find

$$lnZ = \beta N\eta - \frac{9N}{\omega_D^3}\int_0^{\omega_D} ln(1 - e^{-\beta\hbar\omega})\omega^2 d\omega$$

   In terms of dimensionless variables $x = \beta\hbar\omega$ and $y = \beta\hbar\omega_D$ we get

$$lnZ = \frac{yN\eta}{\hbar\omega_D} - \frac{9N}{y^3}\int_0^y ln(1 - e^{-x})x^2 dx = y\frac{N\eta}{\hbar\omega_D} - \frac{9N}{y^3}[ln(1 - e^{-x})x^3/3]_0^y - \frac{1}{3}\int_0^y \frac{x^3 dx}{e^x - 1}$$

$$lnZ = y\frac{N\eta}{\hbar\omega_D} - 3N\ ln(1 - e^{-y}) + ND(y) = \beta N\eta - 3N\ ln(1 - e^{-\theta_D/T}) + N\ D(\theta_D/T)$$

   where $k\theta_D = \hbar\omega_D$

   (b) The mean energy is

$$E = -\frac{\partial}{\partial\beta}lnZ = -\hbar\omega_D\frac{\partial}{\partial y}lnZ = -N\eta + \frac{3N\hbar\omega_D e^{-y}}{1 - e^{-y}} + \frac{9N\hbar\omega_D}{y^4}\int_0^y \frac{x^3 dx}{e^x - 1} - \frac{3N\hbar\omega_D}{y^3}\frac{y^3}{e^y - 1} \Rightarrow$$

$$E = -N\eta + \frac{3N}{\beta}D(y) = -N\eta + 3NkT\ D(\theta_D/T)$$

   (c)

$$S = k(lnZ + \beta E) = Nk[-3ln(1 - e^{-y}) + 4D(y)] = Nk[-3ln(1 - e^{-\theta_D/T}) + 4D(\theta_D/T)]$$

2. Evaluate $D(y)$ in the two limits and use this to calculate the quantities of the previous problem.

   Solution:

   For $y \gg 1$ the upper limit in the integral can be taken to infinity, so

$$D(y) = \frac{3}{y^3}\int_0^\infty \frac{x^3}{e^x - 1} = \frac{\pi^4}{5y^3}$$

   For $y \ll 1$ we expand $e^x \approx 1 + x$ so

$$D(y) = \frac{3}{y^3}\int_0^\eta x^2 dx = 1$$

For the temperature much smaller than the Debye temperature, we get

$$lnZ = \frac{N\eta}{kT} + \frac{N\pi^4 T^3}{5\theta_D^3}$$

$$E = -N\eta + \frac{3\pi^4}{5}\frac{NkT^4}{\theta_D^3}$$

$$S = \frac{4\pi^4}{5}Nk(\frac{T}{\theta_D})^3$$

For the temperature much greater than the Debye temperature, we find using $e^y \approx 1 + y$

$$lnZ = \frac{N\eta}{kT} - 3N\ ln\theta_D/T + N$$

$$E = -N\eta + 3NkT$$

$$S = Nk[-3ln\theta_D/T + 4]$$

3. The expression for the energy of a solid depends in general on the volume. Use the Debye approximation to find the equation of state of the solid, i.e. find the pressure as a function of V and T. What are the limiting cases when $T \ll \Theta_D$ and $T \gg \Theta_D$. Express your answer in terms of the quantity $\gamma = -\frac{V}{\Theta_D}\frac{d\Theta_D}{dV}$

Solution:

$p = \frac{1}{\beta}\frac{\partial}{\partial V}$

$$lnZ = N\frac{\partial\eta}{\partial V} + \frac{3NkTe^{-\theta_D/T}}{1 - e^{-\theta_D/T}}(-\frac{1}{T}\frac{\partial\theta_D}{\partial V}) + NkT[\frac{\partial D(\theta_D/T)}{\partial(\theta_D/T)}][\frac{d(\theta_D/T)}{dV}]$$

where

$$[\frac{\partial D(\theta_D/T)}{\partial(\theta_D/T)}] = -\frac{9}{(\theta_D/T)^4}\int_0^{\theta_D/T}\frac{x^3dx}{e^x - 1} + \frac{3}{e^{\theta_D/T} - 1}$$

$$p = N\frac{\partial\eta}{\partial V} - \frac{3NkT}{\theta_D}D(\theta_D/T)\frac{d\theta_D}{dT}$$

In terms of γ this becomes

$$p = N\frac{\partial\eta}{\partial V} - \frac{3N\gamma kT}{V}D(\theta_D/T)$$

For small T

$$p = N\frac{\partial\eta}{\partial V} + \frac{3\pi^4}{5}\frac{\gamma NkT^4}{V\theta_D^3}$$

For high T

$$p = N\frac{\partial\eta}{\partial V} + \frac{3\gamma NkT}{V}$$

4. Assume that γ is independent of temperature. Show that the coefficient of thermal expansion α is then related to γ by the relation

$$\alpha = \frac{1}{V}\frac{\partial V}{\partial T}|_p = \kappa\frac{\partial p}{\partial T}_V = \kappa\gamma\frac{C_V}{V}$$

where κ is the compressibility

Solution:

$$p = N\frac{\partial \eta}{\partial V} + \gamma\frac{E + N\eta}{V}$$

Thus

$$\alpha = \kappa(\frac{\partial p}{\partial T})_V = \frac{\kappa\gamma}{V}(\frac{\partial E}{\partial T})_V = \kappa\gamma\frac{C_V}{V}$$