

PHSX 671: Homework #7

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Problem 1

Use the Debye approximation to find the expressions for the entropy of a 3-dimensional solid as a function of the temperature T . For simplicity, express your answer in terms of the "Debye Function" $D(y) = \frac{3}{y^3} \int_0^y \frac{x^3}{e^x - 1} dx$ and the "Debye Temperature" $\Theta_D = \frac{\hbar\omega_D}{k_B} = Tx_D$. Assume that each oscillation is independent of the others.

Solution:

$$S = \ln Z - \beta \left(\frac{\partial \ln Z}{\partial \beta} \right) = - \left(\frac{\partial F}{\partial T} \right)$$

$$F = -\frac{1}{\beta} \ln Z$$

I'll choose to do this from the Helmholtz Free energy since it can be done a bit easier. We found:

$$\ln Z = -\frac{9N\beta\hbar\omega}{8} - 3N \ln(1 - e^{-x_D}) - \frac{N}{x_D^3} \int_0^{x_D} \frac{x^3}{e^x - 1} dx$$

$$= -\frac{9Nx_D}{8} - 3N \ln(1 - e^{-x_D}) - ND_3(x_D); \quad x_D = \beta\hbar\omega$$

I'll just keep things in terms of beta, so

$$-\left(\frac{\partial F}{\partial T} \right) = -\left(\frac{\partial F}{\partial \beta} \right) \left(\frac{\partial \beta}{\partial T} \right) = -\left(\frac{\partial F}{\partial \beta} \right) \frac{\partial}{\partial T} \left(\frac{1}{k_B T} \right) = \frac{\beta^2}{k_B} \left(\frac{\partial F}{\partial \beta} \right)$$

Now we can just compute entropy

$$S = -\frac{\partial}{\partial \beta} \left[\frac{1}{\beta} \frac{\beta^2}{k_B} \left(-\frac{9N\beta\hbar\omega}{8} - 3N \ln(1 - e^{-\beta\hbar\omega}) - ND_3(x_D) \right) \right]$$

$$= \frac{\partial}{\partial \beta} \left[\frac{\beta}{k_B} \left(\frac{9N\beta\hbar\omega}{8} + 3N \ln(1 - e^{-\beta\hbar\omega}) + ND_3(x_D) \right) \right]$$

I will assume the form of $\frac{1}{k_B}(U) + \frac{\beta}{k_B}(U')$ (product rule), where U is the contents of the parenthesis. Focusing on the U' term for cleanliness:

$$U' = \frac{\partial}{\partial \beta} \left(\frac{9N\beta\hbar\omega}{8} + 3N \ln(1 - e^{-\beta\hbar\omega}) + ND_3(x_D) \right)$$

$$= \left(\frac{9N\hbar\omega}{8} - 3N\hbar\omega \frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} + N \frac{\partial D_3(x_D)}{\partial \beta} \right)$$

Which gives this beefy equation

$$S = \frac{1}{k_B} \left(\frac{9N\beta\hbar\omega}{8} + 3N \ln(1 - e^{-\beta\hbar\omega}) + ND_3(x_D) \right) + \frac{\beta}{k_B} \left(\frac{9N\hbar\omega}{8} - 3N\hbar\omega \frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} + N \frac{\partial D_3(x_D)}{\partial \beta} \right)$$

And we can tidy it up with the Debye temperature instead of $\hbar\omega$ terms

$$S = \left(\frac{9N\beta\Theta_D}{8} + \frac{3N}{k_B} \ln(1 - e^{-\beta k_B \Theta_D}) + \frac{N}{k_B} D_3(x_D) \right) + \left(\frac{9N\beta\Theta_D}{8} - 3N\beta\Theta_D \frac{e^{-\beta k_B \Theta_D}}{1 - e^{-\beta k_B \Theta_D}} + \frac{N\beta}{k_B} \frac{\partial D_3(x_D)}{\partial \beta} \right)$$

Problem 2

Derive an expression for the pressure of an Einstein solid in terms of $\frac{\partial \omega_0}{\partial V}$. Then use the proportion $\omega_0 \propto V^{-\frac{1}{3}}$ to determine an approximate expression for the pressure of an Einstein solid at $T = 0$.

Solution:

Again I will use Helmholtz Free energy, since it is fewer computations

$$\begin{aligned} \ln Z &= -3N \left[\frac{1}{2}\beta\hbar\omega_0 + \ln(1 - e^{-\beta\hbar\omega_0}) \right] = -3N \left[\frac{1}{2}\beta\hbar\lambda V^{-1/3} + \ln(1 - e^{-\beta\hbar\lambda V^{-1/3}}) \right] \\ P &= \frac{\partial F}{\partial V}; \quad F = -\frac{1}{\beta} \ln Z \end{aligned}$$

I choose to substitute $\omega \rightarrow V^{-1/3}$ times some proportionality constant λ . Differentiating, we get

$$P = \frac{3N}{\beta} \left[\frac{1}{2}\beta\hbar\lambda V^{-4/3} - \frac{\beta\lambda\hbar}{3V^{4/3}} \frac{e^{-\beta\lambda\hbar V^{-1/3}}}{(1 - e^{-\beta\lambda\hbar V^{-1/3}})} \right]$$

Without rigorously proving it, I'll say that the fraction of exponentials converges to zero when $\beta \rightarrow \infty$. This leaves us with a constant pressure at low temperature equal to

$$P = \frac{3N\hbar\lambda V^{-4/3}}{2}$$

Problem 3

Use the Debye approximation to find the expressions for the entropy of a 3-dimensional solid as a function of the temperature T . For simplicity, express your answer in terms of the "Debye Function" $D(y) = \frac{3}{y^3} \int_0^y \frac{x^3}{e^x - 1} dx$ and the "Debye Temperature" $\Theta_D = \frac{\hbar\omega_D}{k_B} = Tx_D$. Assume that each oscillation is independent of the others.

Problem 4

What is the equation of state for a Debye solid? That is, find an expression for the pressure P in terms of the volume V and the temperature T . Express your answer in terms of the "Debye function", $D(y)$, the "Debye temperature", Θ_D , and the Grüneisen parameter, $\gamma = -\frac{V}{\Theta_D} \frac{\partial \Theta_D}{\partial V}$.

Problem 5

A rigid 1-D rod can excite longitudinal normal modes of oscillation down its length, denoted as L . Determine the heat capacity of the rod, C_V , as a function of temperature resulting from these oscillations using a Debye approximation model. Express your answer in terms of an integral and, for the sake of simplicity, consider using the dimensionless variable $x = \beta\hbar\omega$.