Phonon and Harmonic Solid

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Bose-Einstein Distribution and Density of States

Phonons are quantized thermal waves in a solid. Like photon (quantized electromagnetic waves), they obey a wave equation:

$$\nabla^2 \psi = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2}.$$

We already have all ingredients to analyze phonon statistics,

$$\langle n \rangle = \frac{1}{e^{\beta(\epsilon - \mu)} - 1},$$

$$g(\omega) d\omega = 3 \times \frac{V \omega^2}{2\pi^2 v^3} d\omega.$$

Harmonic Solid

At equilibrium, N atoms in a solid can be described by atoms in a harmonic potential (for more details, take solid-state physics course). Therefore, the energy is

$$E = \sum_{i}^{3N} \hbar\omega_i \left(n_i + \frac{1}{2} \right)$$

Since phonons are bosons, we can apply Bose-Einstein statistics with $\mu = 0$ (thermal phonons can be created or destroyed by random energy fluctuations),

$$E = \sum_{i}^{3N} \hbar\omega_i \left(\frac{1}{e^{\beta\hbar\omega_i} - 1} + \frac{1}{2} \right).$$

Einstein Model ($\omega_i = \omega$)

When all modes have the same frequency, we can simply calculate the energy

$$E = \sum_i^{3N} \hbar\omega \left(\frac{1}{e^{\beta\hbar\omega} - 1} + \frac{1}{2} \right)$$
$$= \frac{3N}{2}\hbar\omega + 3N \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1}.$$

When $T \approx 0$ (low temperature),

$$C_v \sim T^{-2} e^{-1/T}.$$

When $T \to \infty$ (high temperature),

$$C_v \sim 3Nk_B.$$

Debye Model

There should be the maximum frequency ω_D due to the smallest wave length as the spacing between atoms. It is impossible for sound waves to propagate through a solid with wavelength smaller than the atomic spacing (frequency larger than $\sim 1/\lambda$. Then,

$$\int_0^{\omega_D} d\omega g(\omega) = \int_0^{\omega_D} d\omega \left(3 \times \frac{V\omega^2}{2\pi^2 v^3}\right) = 3N,$$

and it gives

$$\omega_D = \left(\frac{6N\pi^2 v^3}{V}\right)^{1/3}.$$

Debye Model

The energy is then

$$
\begin{aligned}
E &= \int_0^{\omega_D} d\omega g(\omega)\hbar\omega \left(\frac{1}{e^{\beta\hbar\omega_i}-1}+\frac{1}{2}\right) \\
&= \frac{3V\hbar}{2\pi^2 v^3}\int_0^{\omega_D} d\omega\omega^3 \left(\frac{1}{e^{\beta\hbar\omega_i}-1}+\frac{1}{2}\right) \\
&\approx \frac{3V\hbar}{2\pi^2 v^3}\int_0^{\omega_D} d\omega\frac{\omega^3}{e^{\beta\hbar\omega_i}-1}
\end{aligned}
$$

Letting $x = \beta\hbar\omega$ and $x_D = T_D/T$, we have

$$
E = \frac{3V\hbar}{2\pi^2(\hbar v)^3}(k_B T)^4 \int_0^{T_D/T} d\omega \frac{x^3}{x-1}.
$$

Debye Model

$$E = \frac{3V\hbar}{2\pi^2(\hbar v)^3}(k_B T)^4 \int_0^{T_D/T} d\omega \frac{x^3}{x-1}.$$

When $T \ll T_D$ (low temperature),

$$\int_0^{T_D/T} d\omega \frac{x^3}{x-1} \approx \int_0^{\infty} d\omega \frac{x^3}{x-1} = \frac{\pi^4}{15},$$

$$C_v = \frac{\partial E}{\partial T} \sim T^3.$$

When $T \gg T_D$ (high temperature),

$$\int_0^{T_D/T} d\omega \frac{x^3}{x-1} \approx \int_0^{T_D/T} d\omega (x^2 + \cdots) = \frac{1}{3}\left(\frac{T_D}{T}\right)^3 + \cdots$$

$$C_v = \frac{\partial E}{\partial T} \sim 3Nk_B.$$