# Appendix B: Statistical Physics of a collection of independent harmonic Oscillators+

Why? After solving for phonon dispersion relation, the system becomes a collection of independent oscillators, with frequencies given by $\omega_s(\vec{q})$.

$$Z = \text{Partition function} = \prod_{\text{oscillators } i} \underbrace{z_i}_{} \qquad \text{(B1)}$$

$z_i$: partition function of an oscillator (depends on T)

- For an oscillator with angular frequency $\omega$:

$$z = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+\frac{1}{2})} = \frac{e^{-\frac{\beta\hbar\omega}{2}}}{1-e^{-\beta\hbar\omega}} \qquad \text{(B2)}$$

mean energy

$$\langle e \rangle = -\frac{\partial}{\partial\beta}\ln z = \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{e^{\beta\hbar\omega}-1} \qquad \text{(B3)}$$

$$= \frac{1}{2}\hbar\omega + \langle n \rangle \hbar\omega$$

$$\text{with } \langle n \rangle = \frac{1}{e^{\beta\hbar\omega}-1} \qquad \text{(B4)}$$

$\langle n \rangle$: thermodynamic averaged number of excitations

The form indicates that phonons are bosons and the chemical potential $\mu = 0$

heat capacity

$$C = \frac{k(\beta\hbar\omega)^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2} \qquad \text{(B5)}$$

Helmholtz free energy

$$f = \frac{\hbar\omega}{2} + kT\ln\left(1-e^{-\frac{\hbar\omega}{kT}}\right) = kT\ln\left[2\sinh\left(\frac{\hbar\omega}{2kT}\right)\right] \qquad \text{(B6)}$$

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+ See PHYS4260 Class notes Ch. II.

- Eq. (B4) is particularly important

In a solid at equilibrium at a temperature $T$, the normal mode (OR phonon mode) characterized by $\omega_s(\vec{q})$ is excited to the extent given by

$$\langle n_s(\vec{q})\rangle = \frac{1}{e^{\frac{\hbar\omega_s(\vec{q})}{kT}}-1} \qquad (B7)$$

- The energy of the whole collection of oscillators is

$$E = \underbrace{\sum_s \sum_{\vec{q}\in 1^{st} BZ}}_{\text{sum over all modes}} \left( \frac{\hbar\omega_s(\vec{q})}{2} + \frac{\hbar\omega_s(\vec{q})}{e^{\frac{\hbar\omega_s(\vec{q})}{kT}}-1} \right) \qquad (B8)$$

To do this, turn sums into integral by invoking

$$\underbrace{D(\omega)\,d\omega}_{\#\text{ normal mode frequencies in the interval } \omega \to \omega + d\omega}$$

density of modes
OR density of "states"

- Going back to Eq. (B4):

$$\langle n\rangle = \frac{1}{e^{\beta\hbar\omega}-1}$$

two energies: $\hbar\omega$ vs $kT$

(i) $\hbar\omega \gg kT$

$$\frac{\hbar\omega}{kT} \gg 1, \quad \langle n\rangle \sim e^{-\frac{\hbar\omega}{kT}}$$

(ii) $\hbar\omega \ll kT$

$$\frac{\hbar\omega}{kT} \ll 1 \quad \text{or} \quad e^{\frac{\hbar\omega}{kT}} \approx 1 + \frac{\hbar\omega}{kT}$$

$$\therefore \langle n\rangle \sim \frac{kT}{\hbar\omega}$$

These two limiting behavior are useful in discussing thermal properties of solids.

- Recall (see Appendix A) $\hat{n} = \hat{a}^{+}\hat{a}$

$$\langle n\rangle = \langle \hat{a}^{+}a\rangle$$

$$\left\{ \begin{array}{l} \text{In Stat. mech., we have} \\ \langle \hat{A}\rangle = \dfrac{\sum_i \langle i|\hat{A}|i\rangle e^{-\beta E_i}}{Z} \end{array} \right.$$