Thermal Energy at the Nanoscale

Week 3: Basic Thermal Properties

Lecture 3.1: Introduction to Specific Heat

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A Close Look at Internal Energy

- In general, 'internal' energy is calculated from the sum of energies over all available microstates consisting of
  - Energy of a quantum 'particle'
  - Distribution function (average occupation number) of such particles

Carrier energy (e.g, ħω)

Summations over k-space & polarizations

Distribution function

$$U = \sum_{\mathbf{k}} \sum_{p} E_{i,p}(\mathbf{k}) f_i^o \left[E_{i,p}(\mathbf{k}), T \right]$$

Note: zero-point term neglected (e.g., 1/2 for bosons)

Thermal Energy

- Only the equilibrium distribution function (occupation number) f_i^0 depends on temperature

$$<N_i> = f_i^o = \frac{1}{e^{(E_i - \mu)/k_B T} + \gamma}$$

$$\gamma = 1 \quad (\text{Fermi-Dirac}, i = FD)$$

$$\gamma = -1 \quad (\text{Bose-Einstein}, i = BE)$$

$$\gamma = 0 \quad (\text{Maxwell-Boltzmann}, i = MB)$$

- Form of carrier energy E_i depends on carrier type (fermion, boson)

Sum to Integral Conversion

- **k**-space summation is often cumbersome
- General conversion

$$\lim_{L\to\infty}\frac{1}{L^d}\sum_{\mathbf{k}}F(\mathbf{k}) = \int F(\mathbf{k})\frac{d\mathbf{k}}{(2\pi)^d}$$

  - Where $F(\mathbf{k})$ is a general function in a **k**-space of dimension d
  - Derives from the fact that each allowable state's k-space 'volume' is $(2\pi/L)^d$

Specific Energy

- *Specific* internal energy *u* becomes

$$u = \frac{U}{L^d} = \sum_p \int \frac{E_{i,p}(\mathbf{k}) f_i^o\left[E_{i,p}(\mathbf{k}), T\right]}{(2\pi)^d} d\mathbf{k}$$

Specific Heat

- By definition

Amount of thermal energy required to raise one unit volume (or mass) by one degree

$$c_v = \frac{\partial u}{\partial T} = \sum_p \int \frac{E_{i,p}(\mathbf{k})}{(2\pi)^d} \frac{\partial f_i^o}{\partial T} d\mathbf{k}$$

  – Where

$$\frac{\partial f_i^o}{\partial T} = (f_i^o)^2 e^{(E_i-\mu)/k_B T} \left(\frac{E_i - \mu}{k_B T^2} \right)$$

- **k**-space integrals can still be messy
  – Often converted to energy integrals
  – Use examples to demonstrate