Thermal Energy at the Nanoscale

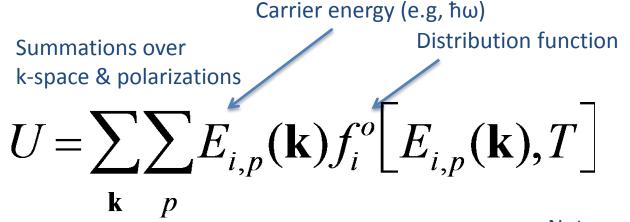
Week 3: Basic Thermal Properties Lecture 3.1: Introduction to Specific Heat

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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



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



 Only the equilibrium distribution function (occupation number) f⁰_i depends on temperature

$$< N_{i} >= f_{i}^{o} = \frac{1}{e^{(E_{i} - \mu)/k_{B}T} + \gamma}$$

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

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

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

• 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(**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 (2π/L)^d



• Specific internal energy u becomes

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



• 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

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