Phys 528 Lecture 8

1) Paramagnetism

$$H = -\sum_{i=1}^{N} \vec{\mu}_i \cdot \vec{B} = -\mu B \sum_{i=1}^{N} \cos\theta_i$$

$$Z_N(\beta) = \left(Z_1(\beta)\right)^N$$

$$Z_1(\beta) = \sum_{\theta} e^{\beta \mu B \cos\theta}$$

$$\vec{B} = B\hat{z}$$

$$M_z = N\langle \mu\cos\theta\rangle = N \frac{\sum_\theta \mu\cos\theta\, e^{\beta\mu B\cos\theta}}{\sum_\theta e^{\beta\mu B\cos\theta}}$$

$$= \frac{N}{\beta}\frac{\partial \ln Z_1}{\partial B} = -\left.\frac{\partial F}{\partial B}\right|_T$$

a) <u>Classical calculation</u>

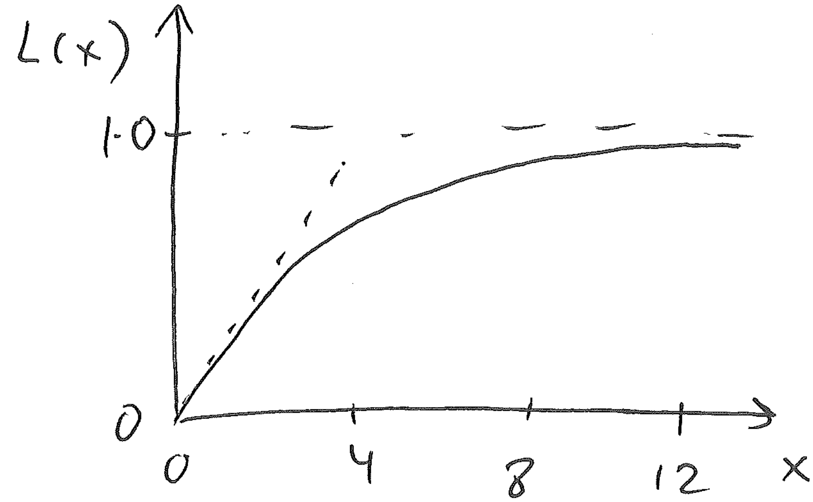
$$Z_1(\beta) = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \, d\theta \; e^{\beta\mu B\cos\theta}$$

$$= \frac{4\pi \sinh(\beta\mu B)}{\beta\mu B}$$

$$\langle \mu_z \rangle = \frac{M_z}{N} = \mu \left\{ \coth(\beta\mu B) - \frac{1}{\beta\mu B} \right\}$$

$$= \mu L(\beta\mu B)$$

$$L(x) = \coth x - \frac{1}{x}$$



N_0 dipoles/volume

$$M_{z0} = N_0 \langle \mu_z \rangle = N_0 \mu L(x)$$

$k_B T \ll \mu B$

$x \gg 1 \qquad L(x) \to 1 \qquad \langle \mu_z \rangle \to \mu$

$$M_{z0} = N_0 \mu \quad \text{(fully polarized)}$$

$k_B T \gg \mu B$

$x \ll 1 \qquad L(x) \simeq \frac{x}{3} - \frac{x^3}{45} + \cdots$

$$M_{z0} \simeq \frac{N_0 \mu^2}{3 k_B T} B$$

$$\chi = \lim_{B \to 0} \left.\frac{\partial M_{z0}}{\partial B}\right|_T = \frac{N_0 \mu^2}{3 k_B T}$$

<u>Curie Law</u>

b) <u>Quantum calculation</u>

$$\vec{\mu} = g\left(\frac{q}{2mc}\right)\vec{L} \qquad q = -e$$

$g = 2$ for spin, $g = 1$ for orbital

$$g = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)} \quad \text{in general}$$

$$\mu^2 = g^2 \mu_B^2 J(J+1) \qquad \mu_B = \frac{e\hbar}{2mc}$$

$$\mu_z = g \mu_B m \, , \quad m = -J, -J+1, \dots, J$$

$$Z_1(\beta) = \sum_{m=-J}^{J} e^{\beta g \mu_B B m}$$

$$= \frac{\sinh\left\{\left(1 + \frac{1}{2J}\right)x\right\}}{\sinh \frac{x}{2J}}$$

$$x = \beta (g \mu_B J) B$$

$$M_z = N\langle \mu_z \rangle = \frac{N}{\beta} \frac{\partial \ln Z_1}{\partial B}$$

$$= N (g \mu_B J) \left\{ \left(1 + \frac{1}{2J}\right) \coth\left\{\left(1 + \frac{1}{2J}\right)x\right\} - \frac{1}{2J} \coth\left(\frac{x}{2J}\right) \right\}$$

$$\langle \mu_z \rangle = g \mu_B J \, B_J(x)$$

$$B_J(x) = \left(1 + \frac{1}{2J}\right) \coth\left\{\left(1 + \frac{1}{2J}\right) x\right\} - \frac{1}{2J} \coth \frac{x}{2J}$$

$k_B T \ll g \mu_B J B \quad (x \gg 1)$

$B_J(x) \to 1$ fully magnetized

$k_B T \gg g \mu_B J B \quad (x \ll 1)$

$$B_J(x) \simeq \frac{1}{3}\left(1 + \frac{1}{J}\right) x + \cdots$$

$$\langle \mu_z \rangle \simeq \frac{(g \mu_B J)^2}{3 k_B T}\left(1 + \frac{1}{J}\right) B$$

$$= \frac{g^2 \mu_B^2 J(J+1)}{3 k_B T} B$$

c.f. Curie Law

2) <u>Negative temperatures</u>

$s = \frac{1}{2}$

$$Z_N(\beta) = \left(e^{\beta\varepsilon} + e^{-\beta\varepsilon}\right)^N$$

$$= \left[2\cosh(\beta\varepsilon)\right]^N, \quad \varepsilon = \mu_B B$$

$$F = -k_B T \ln Z_N = -N k_B T \ln\{2\cosh(\beta\varepsilon)\}$$

$$S = -\frac{\partial F}{\partial T}\Big|_B = N k_B \left[\ln\left\{2\cosh\frac{\varepsilon}{k_B T}\right\} - \frac{\varepsilon}{k_B T}\tanh\frac{\varepsilon}{k_B T}\right\}$$

$$E = -N\varepsilon\tanh(\beta\varepsilon) \le 0 \quad \text{for } \beta > 0$$

$$M = -\frac{\partial F}{\partial B}\Big|_T = N\mu_B\tanh(\beta\varepsilon)$$

$$\frac{1}{T} = -\frac{k_B}{\varepsilon}\tanh^{-1}\left(\frac{E}{N\varepsilon}\right) = \frac{k_B}{2\varepsilon}\ln\left(\frac{N\varepsilon - E}{N\varepsilon + E}\right)$$

$E \to 0$ and $S \to k_B \ln 2$

as $\beta \varepsilon \to 0$ $(T \to \infty)$

But max. possible energy

$$\max\left\{\frac{E}{N}\right\} = +\varepsilon$$

A state with $E \geq 0$

can be assigned a

<u>negative temperature</u>.

Such a state has a population

inversion:

$$\frac{P(\varepsilon)}{P(-\varepsilon)} = \frac{e^{-\beta\varepsilon}}{e^{\beta\varepsilon}} = e^{-\frac{2\varepsilon}{k_B T}} > 1$$

A negative temperature can only be assigned to a system with a spectrum bounded above. cf. Laser physics

<u>2nd Law</u>

$$0 \le \Delta S = \Delta E\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$T_1 \xrightarrow{\Delta E} T_2$$

$$\frac{\Delta S}{k_B} = \Delta E\left(\beta_2 - \beta_1\right)$$

$$\Delta E > 0 \text{ if } \beta_2 > \beta_1$$

If $T_1 < 0$ and $T_2 > 0$ then $\beta_2 > \beta_1$.

Heat flows from a system at negative temperature to one at positive T.

System with negative T is hotter that system with $T \to \infty$, not colder than system with $T = 0$.