Lecture 18 - WiSe2022/2023

Tuesday, December 27, 2022 10:47 AM

2.3. Atomic Paramagnetism

e.g.
- insulator (e.g. MgO, $NaCl$) with a transition metal or a rare earth inside
- Magnetic Molecules
- Color Center in Diamond (Nitrogen-Vacancy-Center)

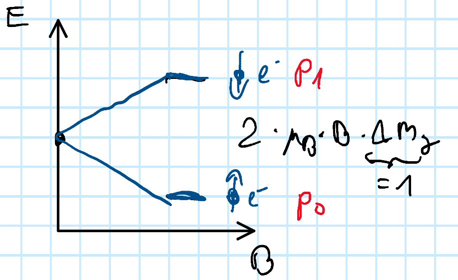
$\hookrightarrow$ no conduction electrons

Landé-factor, total orbital moment

$$E = \mu_B \cdot \vec{B} \, (\vec{L} + g\vec{S})/\hbar = g_J \cdot \mu_B \cdot \frac{\vec{J}}{\hbar} \cdot \vec{B}$$

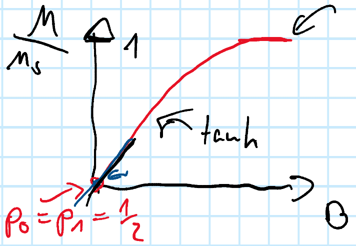
- example: Eigenstates for a spin-$\frac{1}{2}$ system

$J = S = \frac{1}{2} \implies m_J = \pm \frac{1}{2} \qquad g_J = 2$



$$E = -\vec{\mu}_B \cdot \vec{B}$$

$$e^{\left(\frac{\mu_B \cdot B}{k_B T}\right)}$$



reaches M_s, the saturation magnetization
$p_0 = 1$

$p_0 + p_1 = 1$

$$\frac{p_0}{p_1} = e^{-\frac{E}{k_B T}}$$

$$M = \langle m_J \rangle \propto m_0 \cdot p_0 + m_1 \cdot p_1$$

$m_1 = -\frac{1}{2}$

> Lecture on phase transitions
>
> ⚠ the free energy of a finite system is always analytical so non-analyticity can only occur in the thermodynamic limit $N \to \infty$ $\Rightarrow$ Cooperation of all degree of freedom in the system.
>
> Statistical physics $F = k_B T \langle e^{-\mathcal{H}/k_B T} \rangle$ — average over all possible configurations of the system.
>
> Fluctuations are related to susceptibility.
> Magnetic case: $\chi = \left(\frac{\partial m}{\partial h}\right)_T$ — external field
>
> Effect of the magnetic field?

$\}$ Z, the partition function

- Free Energy $F = U - T \cdot S = \ldots = -k_B \cdot T \cdot \ln(Z)$ (p. 669)

$$M = \langle \ldots \rangle = -\frac{\partial F}{\partial B} \ldots \frac{m_{1/2} \cdot e^{x} + m_{-1/2} \cdot e^{-x}}{\ldots} \ldots \frac{e^{x} - e^{-x}}{\ldots}$$

$m_{1/2} = \mu_B$, $m_{-1/2} = -\mu_B$

$$M := \langle m \rangle = -\frac{\partial F}{\partial B} = \frac{\overset{\mu_B}{m_{1/2}} \cdot e^{x} + \overset{-\mu_B}{m_{-1/2}} \cdot e^{-x}}{e^{x} + e^{-x}} \quad \Big\} \quad \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}} = \tanh$$

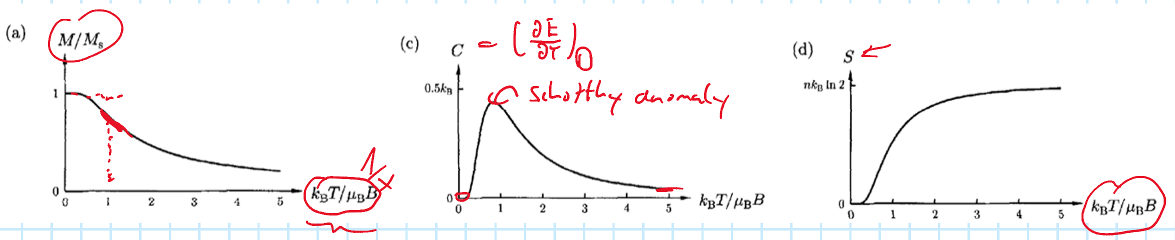
$$x = \frac{\mu_B \cdot B}{k_B T}$$

$$\frac{M}{M_s} = \tanh\left(\frac{\overbrace{\mu_B \cdot B}^{x''}}{k_B \cdot T}\right) \qquad M_s = \max(\langle m \rangle) = \mu_B$$

$$x \ll 1 \to \tanh(x) \approx x$$

Susceptibility $$\chi = \mu_0 \cdot \left(\frac{\partial M}{\partial B}\right)_{T,V} \approx \frac{\mu_0 \cdot \mu_B^2}{k_B T} = \frac{C}{T}$$

$$k_B = 1.38 \cdot 10^{-23}\ \frac{J}{K} = 86\ \frac{\mu eV}{K}$$



$$\langle m_j \rangle = \frac{\sum_{m_j=-1/2}^{m_j=+1/2} m_j \cdot e^{-\frac{m_j \cdot g_j \cdot \mu_B \cdot B}{k_B T}}}{\sum_{m_j=-1/2}^{+1/2} e^{-(m_j \cdot g_j \cdot \mu_B \cdot B)/k_B T}} = -\frac{1}{Z}\frac{\partial Z}{\partial x}$$

$$M = -\overset{n}{\frac{N}{V}} \cdot g_j \cdot \mu_B \cdot \langle m_j \rangle = n\,\frac{g_j \cdot \mu_B}{Z}\,\frac{\partial Z}{\partial B} \cdot \frac{\partial B}{\partial x}$$

$$= n \cdot k_B \cdot T \cdot \frac{\partial \ln Z}{\partial B} \qquad Z = \frac{\sinh\left[(2J+1) \cdot \frac{x}{2}\right]}{\sinh\left(\frac{x}{2}\right)}$$

Brillouin function

$$\frac{M}{M_s} = B_J(y) = \frac{2J+1}{2J} \cdot \coth\left(\frac{2J+1}{2J} \cdot y\right) - \frac{1}{2J} \cdot \coth\left(\frac{1}{2J} \cdot y\right)$$

$$y = x \cdot J = \frac{g_J \cdot \mu_B \cdot J \cdot B}{k_B \cdot T}$$

$$M_s = n \cdot g_J \cdot \mu_B \cdot J$$

$$B_J(y) \simeq \frac{J+1}{3J} \cdot y = \frac{J+1}{3} \cdot x$$

$$\chi = \mu_0 \cdot \left(\frac{\partial M}{\partial B} \right)_{T,V} = \frac{\mu_0 \cdot n \cdot J(J+1)\, g_J^2 \cdot \mu_B^2}{3\, k_B T} = \frac{C}{T}$$

$$C = \frac{\mu_0 \cdot n \cdot (p \cdot \mu_B)^2}{3\, k_B} = \frac{\mu_0 \cdot n \cdot \mu_{eff}^2}{3 k_B}$$

effective magneton number $p = g_J \sqrt{J(J+1)}$

$\mu_{eff} = p \cdot \mu_B$