TD 6

Ex 2 : Electrons piégés

A sites discernables : $\varepsilon_\uparrow = -\varepsilon_0 \quad \varepsilon_\downarrow = -\varepsilon_0$

$\varepsilon_{\uparrow\downarrow} = -2\varepsilon_0 + g$

1/ Energie du système dans config L : $E_L = \sum_{i=1}^{A} \varepsilon_i$ avec $\varepsilon_i = \begin{cases} 0 \\ -\varepsilon_0 \\ -\varepsilon_0 \\ -2\varepsilon_0 + g \end{cases}$

→ A syst indép.

$$\xi_A = \sum_{\{\ell\}} e^{-\beta(E_\ell - \mu N_\ell)} = 1 + e^{+\beta(\varepsilon_0+\mu)} + e^{+\beta(\varepsilon_0+\mu)} + e^{+\beta(2\varepsilon_0 - g + 2\mu)}$$

nb moyen d'électrons piégés sur un site :

$$\bar{n} = \sum_{\{\ell\}} N_\ell \, p_\ell = \frac{1}{\xi_A} \sum_{\{\ell\}} N_\ell \, e^{-\beta(E_\ell - \mu N_\ell)}$$

$$= \frac{1}{\xi_A}\frac{1}{\beta}\frac{\partial \xi_A}{\partial \mu} = \frac{1}{\beta}\frac{\partial \ln \xi_A}{\partial \mu}$$

$$= \frac{2e^{\beta(\varepsilon_0+\mu)} + 2e^{\beta(2\varepsilon_0 - g + 2\mu)}}{\xi_A}$$

$$= \frac{2e^{\beta(\varepsilon_0+\mu)} + 2e^{2\beta(\varepsilon_0+\mu)}e^{-\beta g}}{\xi_A}$$

→ nb moyens d'e⁻ piégés $\bar{N} = A\,\bar{n}$

2/ $\bar{N} = A$ (équivalence ensemble grand canonique – canonique)

$\Leftrightarrow \bar{n} = 1$

$\Leftrightarrow 1 + \cancel{2e^{\beta(\varepsilon_0+\mu)}} + e^{2\beta(\varepsilon_0+\mu)}e^{-\beta g} = \cancel{2e^{\beta(\varepsilon_0+\mu)}} + 2e^{2\beta(\varepsilon_0+\mu)}e^{-\beta g}$

$\Leftrightarrow 1 = e^{2\beta(\varepsilon_0+\mu)}e^{-\beta g}$

$\Leftrightarrow 0 = \beta(2\varepsilon_0 + 2\mu - g) \quad \Leftrightarrow \boxed{\mu = \frac{g}{2} - \varepsilon_0}$

Proba qu'un site donné soit vide : $P_0 = \sum_{\{\ell\}, N_\ell = 0} p_\ell = \frac{1}{\xi_A} \quad \rightarrow \bar{N}_0 = \frac{A}{\xi_A}$

——— contienne 1 e⁻ : $P_1 = \sum_{\{\ell\}, N_\ell = 1} p_\ell = \frac{2e^{\beta(\varepsilon_0+\mu)}}{\xi_A} \rightarrow \bar{N}_1 = \frac{2A\,e^{\beta(\varepsilon_0+\mu)}}{\xi_A}$

——— 2 e⁻ : $P_2 = \frac{e^{\beta(2\varepsilon_0 + 2\mu - g)}}{\xi_A} \rightarrow \bar{N}_2 = A\,e^{2\beta(\varepsilon_0+\mu)}e^{-\beta g}/\xi_A$

si $\mu = \frac{g}{2} - \varepsilon_0 \rightarrow \xi_A = 1 + 2e^{\frac{\beta g}{2}} + 1$

$$= 2\left(1 + e^{\frac{\beta g}{2}}\right)$$

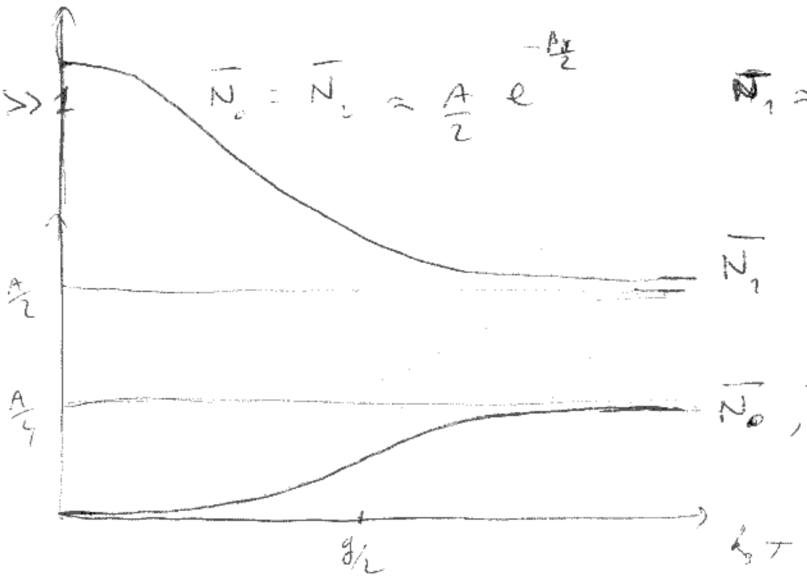
$\Rightarrow \overline{N_0} = \frac{A}{2(1+e^{\beta g/2})}$ | $\overline{N_1} = \frac{\cancel{2} A e^{\beta g/2}}{\cancel{2}(1+e^{\beta g/2})} = \frac{A}{1+e^{-\beta g/2}}$ | $\overline{N_2} = \frac{A}{2(1+e^{\beta g/2})} \ (= \overline{N_0})$

- qd $\frac{\beta g}{2} << 1$ $\quad \overline{N_0} = \frac{A}{4}$, $\overline{N_1} = \frac{A}{2}$, $\overline{N_2} = \frac{A}{4}$

+ précisément, $e^{\frac{\beta g}{2}} = 1 + \frac{\beta g}{2} + \mathcal{O}\left(\left(\frac{\beta g}{2}\right)^2\right) \rightarrow \overline{N_0} = \frac{A}{4(1+\frac{\beta g}{4})} \simeq \frac{A}{4}\left(1 - \frac{\beta g}{4}\right) = \overline{N_2}$

$$\overline{N_1} = \frac{A}{2}\left(1 + \frac{\beta g}{4}\right)$$

- qd $\frac{\beta g}{2} >> 1$ $\quad \overline{N_0} = \overline{N_2} \simeq \frac{A}{2} e^{-\frac{\beta g}{2}}$ $\quad \overline{N_1} \simeq A\left(1 - e^{-\frac{\beta g}{2}}\right)$



3/ Solide sous champ $\vec{B}$.

$\rightarrow \varepsilon_\uparrow = -\varepsilon_0 - mB \qquad \varepsilon_\downarrow = -\varepsilon_0 + mB \qquad \varepsilon_{\uparrow\downarrow} = -2\varepsilon_0 + g$

(a) $\rightarrow \xi_A = \sum_{\{\ell\}} e^{-\beta(\varepsilon_\ell - \mu N_\ell)} = 1 + e^{\beta(\varepsilon_0 + mB + \mu)} + e^{\beta(\varepsilon_0 - mB + \mu)} + e^{+\beta(2\varepsilon_0 - g + 2\mu)}$

Moment moyen d'un site

$$\langle \mu_z \rangle = m \times \frac{e^{\beta(\varepsilon_0 + mB + \mu)}}{\xi_A} - m\frac{e^{\beta(\varepsilon_0 - mB + \mu)}}{\xi_A}$$

$$\boxed{\langle m_z \rangle = m \frac{e^{\beta(\varepsilon_0 + \mu)}}{\xi_A} 2\,\mathrm{sh}(\beta m B)}$$

Aimantation :
$M = \frac{A}{V}\langle m_z \rangle$

(b) $\bar{N} = A \iff ?$

$$\bar{n} = \sum_{\{l\}} N_l P_l = \frac{1}{\xi_A}\left(1 + e^{\beta(\varepsilon_0 + mB + \mu)} + e^{\beta(\varepsilon_0 - mB + \mu)} + 2e^{\beta(2\varepsilon_0 - g + 2\mu)}\right)$$

$$\bar{n} = 1 \iff 1 = e^{\beta(2\varepsilon_0 - g + 2\mu)}$$

$$\iff \boxed{\mu = \frac{g}{2} - \varepsilon_0} \quad \text{(comme précédemment)}$$

$$\Rightarrow \xi_A = 1 + e^{\beta(\frac{g}{2} + mB)} + e^{\beta(\frac{g}{2} - mB)} + 1$$

$$\boxed{\xi_A = 2\left(1 + e^{\frac{\beta g}{2}} ch(\beta mB)\right)}$$

et $$\langle m_z \rangle = m \frac{\left[e^{\beta(\frac{g}{2} + mB)} - e^{\beta(\frac{g}{2} - mB)}\right]}{\xi_A}$$

$$\boxed{\langle m_z \rangle = \frac{m\, e^{\frac{\beta g}{2}} sh(\beta mB)}{1 + e^{\frac{\beta g}{2}} ch(\beta mB)}} \quad , \quad \text{et } M = \frac{A}{V}\langle m_z \rangle$$