

Ferromagnétisme:

7.1 Modèle de Hubbard

1. Sol. $U=0$ sans int.
2. Sol. $t=0$ élec. libres

7.2 $U \ll t$ bande faiblement remplie Ferrom.

1. Stoner
2. $|\Psi\rangle$ variationnelle
3. $-T \ln Z < -T \ln Z_0 + \langle H - H_0 \rangle_0$
4. Eq. du gap. Div. Landau (L.-G.)
5. G

7.1. Modèle de Hubbard:

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Sur réseau

Hubbard Gutzwiller
Kanamori

$$H = - \sum_{ij} \sum_{\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{U}{2} \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i-\sigma}^{\dagger} c_{i-\sigma} c_{i\sigma}$$

$$t_{ij} = t_{ji}^*$$

1 bande.

$$c_{i\sigma} c_{i\sigma} = 0$$

i dénote site sur lequel l'état de Wannier est "localisé"

$$= K + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$U=0, \quad t_{ij} \neq 0 \quad i \text{ et } j \text{ premiers voisins.}$

$$H_0 = -t \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma})$$

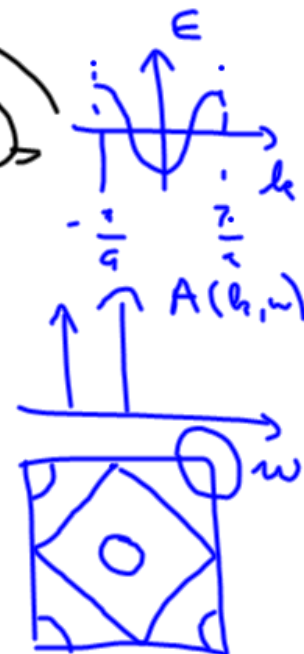
$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k}\sigma}$$

$$\sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} = N \delta_{\mathbf{k},0}$$

$$H_0 = -2t \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$$

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a)$$

$$\mathcal{G}(\mathbf{k}, i\hbar_n) = \frac{1}{i\hbar_n - \epsilon_{\mathbf{k}} + \mu}$$



2. Limite atomique: $t=0$

$$H_1 = NU n_\uparrow n_\downarrow$$

$$\rightarrow Z = 1 + e^{-\beta(-\mu) - \beta(-\mu)} + e^{-\beta(U - 2\mu)}$$

Sans. int:

$$Z = (1 + e^{\beta\mu})(1 + e^{\beta\mu})$$

$$Q(\tau) = - \langle T_\tau c_\sigma(\tau) c_\sigma^\dagger \rangle$$

$$\sum_m |m\rangle \langle m|$$

$$\left. \begin{array}{l} E_0 = 0 \\ E_1 = U \end{array} \right\} \begin{array}{l} n_\uparrow = n_\downarrow = 0 \\ n_\uparrow = 0 \\ n_\downarrow = 1 \\ n_\uparrow = 1 \\ n_\downarrow = 0 \\ n_\uparrow = n_\downarrow = 1 \end{array}$$

Eqs. du mt:

$$K = H_1 - \mu N$$

$$\frac{\partial G_\sigma(\tau)}{\partial \tau} = -\delta(\tau) - \langle T_\tau [K, c_\sigma(\tau)] c_\sigma^\dagger \rangle$$

$$= -\delta(\tau) + \mu G_\sigma(\tau) + U G_{2,\sigma}(\tau)$$

$$(i\omega_n + \mu) G_\sigma(i\omega_n) = 1 + U G_{2,\sigma}(i\omega_n)$$

$$G_{2,\sigma} = \langle T_\tau c_\sigma n_{-\sigma} c_\sigma^\dagger(-\tau) \rangle$$

$$\frac{\partial}{\partial \tau} G_{2,\sigma}(\tau) = \delta(\tau) \langle n_{-\sigma} \rangle + \mu G_{1,\sigma}(\tau) + U G_{2,\sigma}(\tau)$$

$$(i\omega_n + \mu) G_{2,\sigma} = \langle n_{-\sigma} \rangle + U G_{2,\sigma}$$

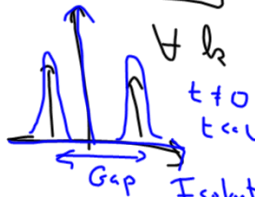
$$G_{2,\sigma} = \frac{\langle n_{-\sigma} \rangle}{i\omega_n + \mu - U}$$

$$G_\sigma(i\omega_n) = \frac{1}{i\omega_n + \mu} \left[1 + \frac{U \langle n_{-\sigma} \rangle}{i\omega_n + \mu - U} \right]$$

$$\frac{1}{i\omega_n + \mu - U} \frac{1}{i\omega_n + \mu} = \frac{1}{U} \left[\frac{1}{i\omega_n + \mu - U} - \frac{1}{i\omega_n + \mu} \right]$$

$$G_\sigma(i\omega_n) = \frac{1 - \langle n_{-\sigma} \rangle}{i\omega_n + \mu} + \frac{\langle n_{-\sigma} \rangle}{i\omega_n + \mu - U}$$

$$G_\sigma^R(\omega) \rightarrow A(\hbar, \omega)$$



$$\langle n_{-\sigma} \rangle = 1/2, \mu = U/2$$

$$G_\sigma^R(\omega) = \frac{1}{2} \left[\frac{1}{\omega + i\eta + U/2} + \frac{1}{\omega + i\eta - U/2} \right]$$

$$= \frac{(\omega + i\eta)}{(\omega + i\eta)^2 - (U/2)^2} = \frac{1}{(\omega + i\eta) - \frac{U^2}{4(\omega + i\eta)}}$$

$$\sum^R(\omega) = \frac{U^2}{4(\omega + i\eta)}$$

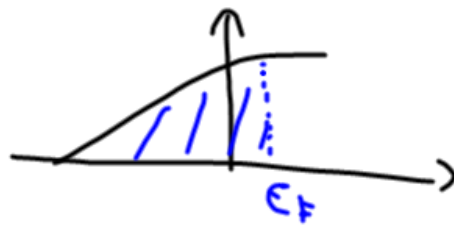
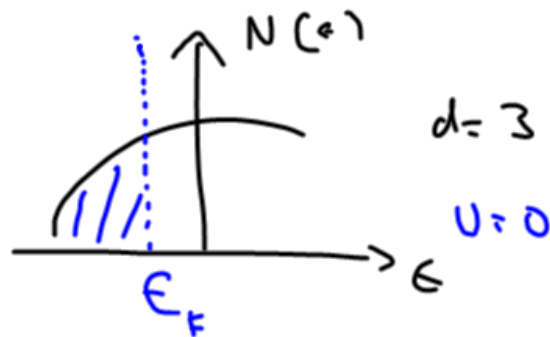
7.2 Modèle de Stoner, Ferromagn.



$$E_{h\uparrow} = E_h + U \langle n_{\downarrow} \rangle$$

$$E_{h\downarrow} = E_h + U \langle n_{\uparrow} \rangle$$

"Weiss"



$$H_{S.B.} = H + h (\langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle) N$$

↑ infinitésimal

$h \rightarrow 0$

$h \rightarrow 0$ en premier

$N \rightarrow \infty$ et $h \rightarrow 0$

$N \rightarrow \infty$
~



g. Fonction d'onde:

$$|\Psi\rangle = \prod_{k\uparrow} \theta(k_{F\uparrow} - |k|)$$

$$\prod_{k\downarrow} \theta(k_{F\downarrow} - |k|) c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger |0\rangle$$

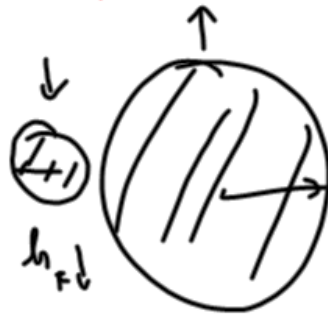
$$k_{F\uparrow} \neq k_{F\downarrow}$$

$$K = H - \mu N$$

Ritz: $\langle n_\uparrow \rangle \neq \langle n_\downarrow \rangle$

$$\frac{\langle \Psi | K | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

doit être
minimisé



$k_{F\uparrow}$

$$|\Psi\rangle = |FS_\uparrow\rangle |FS_\downarrow\rangle$$

7.2.3 Princ. variationnel de Feynmann

$$-T \ln Z \leq -T \ln Z_0 + \langle H - H_0 \rangle_0$$

$$\tilde{H}_0 = \sum_{h\sigma} \tilde{\epsilon}_{h\sigma} c_{h\sigma}^\dagger c_{h\sigma}$$

$$\tilde{H}_1 = \sum_{h\sigma} \epsilon_{h\sigma} c_{h\sigma}^\dagger c_{h\sigma} + U \sum_i \langle n_{i\downarrow} \rangle c_{i\uparrow}^\dagger c_{i\uparrow} + U \sum_i \langle n_{i\uparrow} \rangle c_{i\downarrow}^\dagger c_{i\downarrow}$$

$$\tilde{\epsilon}_{h\uparrow} = \epsilon_{h\uparrow} + U \langle n_{h\downarrow} \rangle$$

$$\tilde{\epsilon}_{h\downarrow} = \epsilon_{h\downarrow} + U \langle n_{h\uparrow} \rangle$$

$$\sum_i c_{i\uparrow}^\dagger c_{i\uparrow} = \sum_h c_{h\uparrow}^\dagger c_{h\uparrow}$$

$$\begin{aligned}
& -T \ln Z_{\vec{v}} + \langle H \cdot \bar{H} \rangle_{\vec{0}} \\
& = -T \ln \left[\prod_h \left(1 + e^{-\beta(\epsilon_h + U \langle n_{\downarrow} \rangle - \mu)} \right) \right. \\
& \quad \left. \prod_h \left(1 + e^{-\beta(\epsilon_h + U \langle n_{\uparrow} \rangle - \mu)} \right) \right] \\
& \quad + U \langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle N - 2U \langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle N
\end{aligned}$$

$$\begin{aligned}
 & -T \sum_k \ln(1 + e^{-\beta(\epsilon_k + U \langle n_\downarrow \rangle)}) \\
 & -T \sum_k \ln(1 + e^{-\beta(\epsilon_k + U \langle n_\uparrow \rangle)}) \\
 \hline
 & \boxed{\epsilon_k = \epsilon_{k-m}} \qquad -NU \langle n_\uparrow \rangle \langle n_\downarrow \rangle
 \end{aligned}$$

def: $m = \langle n_\uparrow \rangle - \langle n_\downarrow \rangle$

$n = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle$

~~$+T \sum_k \frac{e^{-\beta(\epsilon_k + U \langle n_\downarrow \rangle)}}{1 + e^{-\beta(\epsilon_k + U \langle n_\downarrow \rangle)}} \left(-NU \frac{\partial \langle n_\downarrow \rangle}{\partial m} \right)$~~

$+ \langle n_\downarrow \rangle \leftrightarrow \langle n_\uparrow \rangle$

~~$-UN \frac{\partial \langle n_\uparrow \rangle}{\partial m} \langle n_\downarrow \rangle - UN \langle n_\uparrow \rangle \frac{\partial \langle n_\downarrow \rangle}{\partial m} = 0$~~

$= -\sum_k f(\epsilon_k + U \langle n_\downarrow \rangle) + \sum_k f(\epsilon_k + U \langle n_\uparrow \rangle)$

$-N(\langle n_\downarrow \rangle - \langle n_\uparrow \rangle) = 0$

$\langle n_\uparrow \rangle - \langle n_\downarrow \rangle = \frac{1}{N} \sum_k \underbrace{f(\epsilon_k + U \langle n_\downarrow \rangle)}_{\leftarrow} - \underbrace{f(\epsilon_k + U \langle n_\uparrow \rangle)}_{\leftarrow}$

$\langle n_\uparrow \rangle + \langle n_\downarrow \rangle = n = \quad +$

7.2.4 Equation au gap (Landau)

$$m = \frac{1}{N} \sum_k \left[f(\rho_k + U(\frac{n}{2} - \frac{m}{2})) - f(\rho_k + U(\frac{n}{2} + \frac{m}{2})) \right]$$

$$n = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle$$

$$m = \langle n_\uparrow \rangle - \langle n_\downarrow \rangle$$

Soit $m \ll n$

$$\begin{aligned} m &= \frac{1}{N} \sum_k \frac{\partial f}{\partial \rho_k} (-Um) + \mathcal{O}(m^3) \\ &= \int \frac{d^3 k}{(2\pi)^3} \frac{\partial f}{\partial \rho_k} (-Um) + \mathcal{O}(m^3) \end{aligned}$$

$$m = N(E_F) U m + b m^3$$

$$m^2 = \frac{1}{b} (1 - UN(E_F))$$

$$b < 0$$

$$\text{Si } 1 - UN(E_F) < 0$$

$$1 = UN(E_F)$$

$$m \neq 0$$

où m devient $\neq 0$

Critère de Stoner

Si calcule $-T \ln Z$ en puissances de m :

$$F = -\frac{1}{2} (1 - N(E_F)U) m^2 + \frac{b}{4} m^4$$

$m =$ paramètre d'ordre

Champ
moyen

$$F = -\frac{1}{2} a m^2 + \frac{b}{4} m^4$$

$$\frac{\partial F}{\partial m} = 0$$

Ginzburg-Landau

Argument simple pour Stoner:

$$\left. \begin{aligned} E_{h_{F\uparrow}} + U \langle n_{\downarrow} \rangle &= \mu \\ E_{h_{F\downarrow}} + U \langle n_{\uparrow} \rangle &= \mu \end{aligned} \right\} \text{Normal.}$$

$$\rightarrow E_{h_{F\uparrow}} - E_{h_{F\downarrow}} = -U (\langle n_{\downarrow} \rangle - \langle n_{\uparrow} \rangle)$$

$$\frac{\partial E_{h_F}}{\partial h_F} \frac{\partial h_F}{\partial n} (\langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle) = U (\langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle)$$

$$\frac{\partial E_{h_F}}{\partial n} = U$$

Critère
de Stoner

$$1 = U \frac{\partial n}{\partial E_{h_F}} = U N(E_F)$$

7.9.5 Fonctions de Green
"Milieu effectif"

$$\tilde{H}_0 = \sum_{k\sigma} \tilde{\epsilon}_{k\sigma} c_{k\sigma}^+ c_{k\sigma}$$

$$\sum_{\sigma} \tilde{\epsilon}_{k\sigma} = \begin{matrix} \circlearrowleft n_{-\sigma} \\ \vdots \\ \epsilon_{k\sigma} - \tilde{\epsilon}_{k\sigma} \\ \vdots \end{matrix} + \dots$$

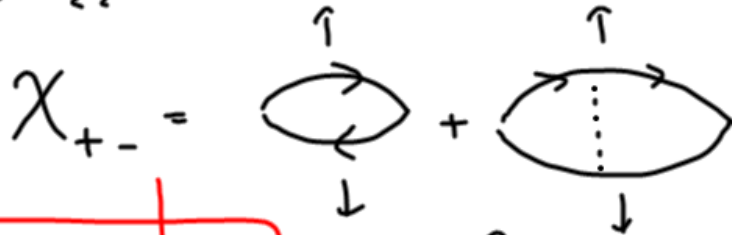
$$\rightarrow \boxed{\sum_{\sigma} \tilde{\epsilon}_{k\sigma} = U \langle n_{-\sigma} \rangle + \epsilon_{k\sigma} - \tilde{\epsilon}_{k\sigma} = 0}$$

$$\tilde{\epsilon}_{k\sigma} = \epsilon_{k\sigma} + U \langle n_{-\sigma} \rangle$$

$$g_{\sigma}(k, i\hbar\omega) = \frac{1}{i\hbar\omega - \tilde{\epsilon}_{k\sigma} + \mu}$$

$$\begin{aligned} \langle n_{\sigma} \rangle &= \sum_k \langle c_{k\sigma}^+ c_{k\sigma} \rangle \\ &= \sum_k - \langle T_{\tau} c_{k\sigma}(\tau=0^-) c_{k\sigma} \rangle \\ &= \sum_k T \sum_n e^{i\hbar\omega n} \frac{1}{i\hbar\omega - \tilde{\epsilon}_{k\sigma} + \mu} \end{aligned} \quad 0^- \equiv \eta$$

$$\boxed{\langle n_{\sigma} \rangle = \sum_k f(\tilde{\epsilon}_{k\sigma} - \mu)}$$

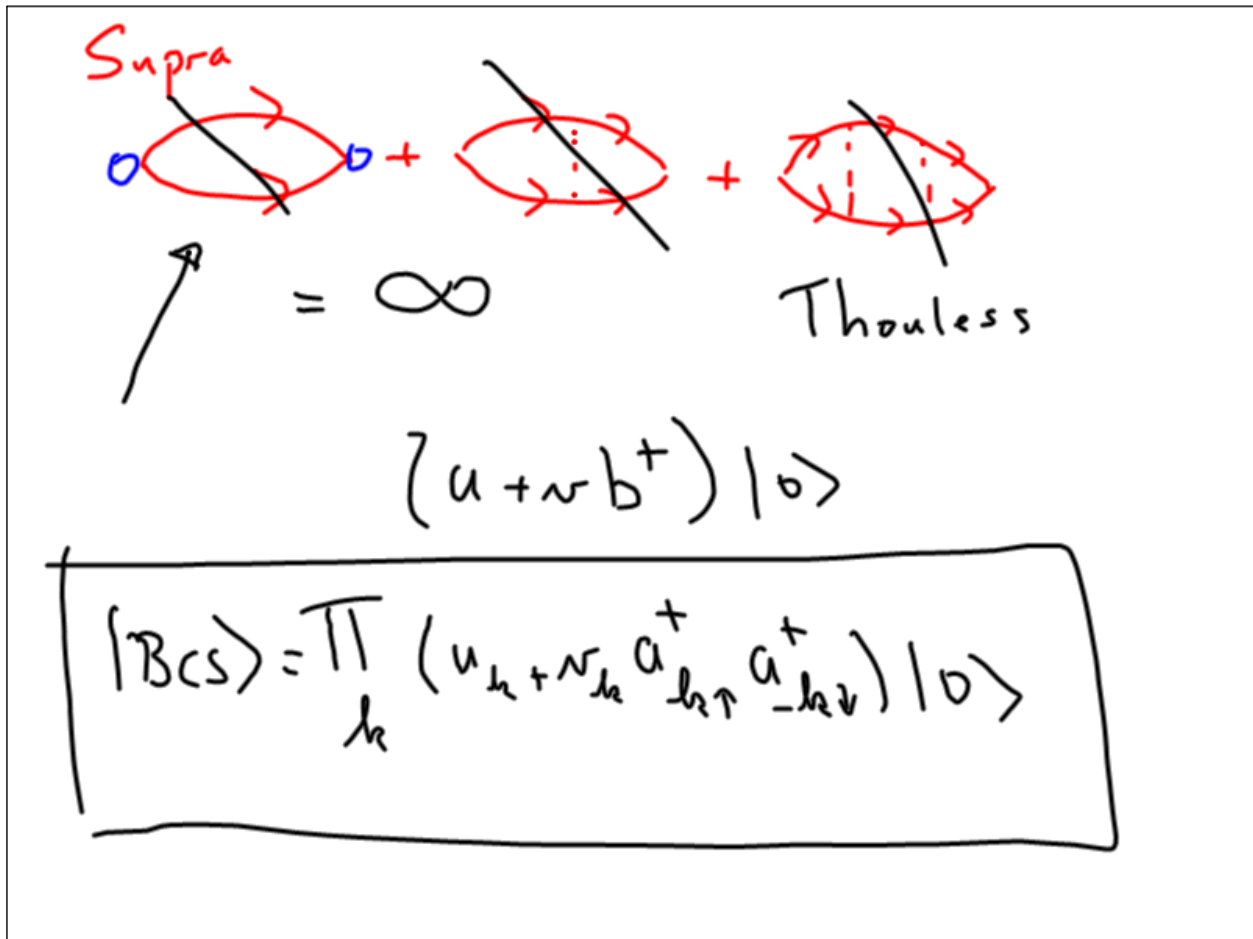
χ_{z_2} 

$$1 = \frac{U}{2} \chi^0(\mathbb{g}, 0)$$

$$\frac{\chi^0}{1 - \frac{U}{2} \chi^0}$$

$$1 - \frac{U}{2} \chi^0 = 0$$

$$\chi^0(\mathbb{g}=0, \omega) = 2N(\mathbb{F}_p)$$



$$\sum_{\substack{k, k' \\ \sigma, \sigma'}} c_{k\sigma}^+ c_{k'\sigma'}^+ c_{k+q, \sigma'} c_{k\sigma}$$

$q=0$

$$\sum_{k'} \langle c_{k'\sigma'}^+ c_{k'\sigma'} \rangle = \langle n_{\sigma'} \rangle$$

Supra

$$\sum_k \langle c_{k\sigma}^+ c_{-k-\sigma}^+ \rangle \neq 0$$

$$k+q = -k \quad \sigma' = -\sigma$$

$$\tilde{H}_0 = c^\dagger c + c_z^\dagger c_z^\dagger + c_r c_r$$

$$\left(\Psi_n \right)_{\text{nambu}} = \begin{pmatrix} c_{h\uparrow} \\ c_{-h\downarrow}^\dagger \end{pmatrix}$$

$$\rightarrow \left\{ \Psi_{h\alpha}, \Psi_{h'\beta}^\dagger \right\} = \delta_{hh'} \delta_{\alpha\beta}$$

$$\tilde{H}_0 = \Psi^\dagger M \Psi$$