45. Modèle de Hubbard

1. "Dérivation" ✓
2. Cas $U=0$ ✓
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46. Modèle de Hubbard dans les traces du gaz d'électrons ✓

1. Propriétés à 1 corps ✓
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4. RPA + viol du principe de Pauli ✓
5. RPA + transitions de phase + Mermin-Wagner ✓

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45. Modèle de Hubbard

1. "Dérivation"

$\langle i|$ Base de Wannier

$|\psi\rangle = c^\dagger_{k_1} c^\dagger_{k_2} \cdots |0\rangle$

$$\mathcal{H} = \sum_{ij\sigma} c^\dagger_{i\sigma} \overbrace{\langle i|\hat{T}+\hat{V}_\ell|j\rangle}^{-t_{ij}} c_{j\sigma}$$

$$+ \frac{1}{2}\sum_{\substack{ijkl\\ \sigma\sigma'}} c^\dagger_{i\sigma} c^\dagger_{j\sigma'} \underbrace{\langle i|\langle j|\hat{V}_c|k\rangle|l\rangle}_{U} c_{l\sigma'} c_{k\sigma}$$

$= 0$ si diagonalisé

$$H = -\sum_{\substack{ij\\ \sigma}} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{1}{2} U \sum_{\substack{i\\ \sigma\sigma'}} c^{\dagger}_{i\sigma} c^{\dagger}_{i\sigma'} c_{i\sigma'} c_{i\sigma}$$

$$= \frac{1}{2} U \sum_{i\sigma} c^{\dagger}_{i\sigma} c^{\dagger}_{i-\sigma} c_{i-\sigma} c_{i\sigma}$$

$$= \frac{1}{2} U \sum_{i\sigma} c^{\dagger}_{i\sigma} c_{i\sigma} c^{\dagger}_{i-\sigma} c_{i-\sigma}$$

$$= U \sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad \boxed{n_{i\uparrow} = c^{\dagger}_{i\uparrow} c_{i\uparrow}}$$

Hubbard

$$\boxed{K = -\sum_{ij} t_{ij}\, c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma}}$$

45.2 Cas $U=0$

$$-\sum_{\substack{ij\\ \sigma}} c^{\dagger}_{i\sigma} t_{ij} c_{j\sigma} = \frac{-1}{N} \sum_{\substack{i,\sigma\\ \delta}} \sum_{k} \sum_{k'} e^{-ik'\cdot r_i} c^{\dagger}_{k'\sigma} t_{\delta} e^{ik\cdot(r_i+\delta)} c_{k\sigma}$$

$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{k} e^{ik\cdot r_i} c_{k\sigma} \qquad V = Na^3 \quad \text{avec} \quad a=1$$

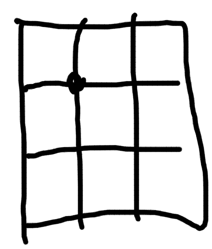
$$\sum_{i} e^{ik\cdot r_i} = N\delta_{k,0} \qquad = -\sum_{k\sigma} c^{\dagger}_{k\sigma} c_{k\sigma} \left(\sum_{\delta} e^{ik\cdot\delta} t_{\delta} \right)$$

$$= \sum_{k\sigma} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} \quad \text{où} \quad \epsilon_k = -\sum_{\delta} e^{ik\cdot\delta} t_{\delta}$$

exemple: réseau carré $d=2$

Sauts (hopping) premier voisin $t_{\delta} = t$ pour δ premier voisin

$$\epsilon_k = -2t(\cos k_x + \cos k_y)$$



45.3 Cas $t=0$

$$K = U\sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma} = \sum_i K_i$$

$$Z = \left[Z_1 \right]^N \qquad \boxed{K_i = U n_\uparrow n_\downarrow - \mu (n_\uparrow + n_\downarrow)}$$

$$Z_1 = \mathrm{Tr}\, e^{-\beta K_1} = 1 + e^{\beta\mu} + e^{\beta\mu} + e^{-\beta(U-2\mu)}$$

si $U=0$

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

Dynamique :

$$\mathcal{G}_\sigma(\tau) = -\langle T_\tau\, c_\sigma(\tau)\, c_\sigma^+ \rangle$$

$$\frac{\partial c_\sigma(\tau)}{\partial \tau} = [K, c_\sigma(\tau)]$$

$$[U n_\sigma n_{-\sigma} - \mu n_\sigma, c_\sigma]$$

$$= [U n_\sigma, c_\sigma]\, n_{-\sigma}$$

$$-\mu [n_\sigma, c_\sigma]$$

$$= -U c_\sigma n_{-\sigma} + \mu c_\sigma$$

$$\frac{\partial \mathcal{G}_\sigma(\tau)}{\partial \tau} = -\delta(\tau) - \langle T_\tau \frac{\partial c_\sigma(\tau)}{\partial \tau} c_\sigma^+ \rangle$$

$$= -\delta(\tau) + U \langle T_\tau\, c_\sigma(\tau)\, n_{-\sigma}(\tau)\, c_\sigma^+ \rangle$$

$$-\mu \langle T_\tau\, c_\sigma(\tau)\, c_\sigma^+ \rangle$$

$$\mathcal{G}_{2\sigma}(\tau) \equiv - \langle T_\tau\, c_\sigma(\tau)\, n_{-\sigma}(\tau)\, c_\sigma^+ \rangle$$

$$\frac{\partial n_{-\sigma}(\tau)}{\partial \tau} = 0$$

① → $$\boxed{\frac{\partial \mathcal{G}_\sigma(\tau)}{\partial \tau} = -\delta(\tau) + \mu \mathcal{G}_\sigma(\tau) - U \mathcal{G}_{2\sigma}(\tau)}$$

② → $$\boxed{\frac{\partial \mathcal{G}_{2\sigma}(\tau)}{\partial \tau} = -\delta(\tau)\langle n_{-\sigma}\rangle + \mu \mathcal{G}_{2\sigma}(\tau) - U \mathcal{G}_{2\sigma}(\tau)}$$

①

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

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

$$\mathcal{G}_{2\sigma}(i\omega_n) = \frac{\langle n_{-\sigma}\rangle}{i\omega_n + \mu - U}$$

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

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

$$\mathcal{G}_\sigma(i\omega_n) = \frac{1 - \langle n_{-\sigma}\rangle}{i\omega_n + \mu} + \frac{\langle n_{-\sigma}\rangle}{i\omega_n + \mu - U}$$ indépendant de $\vec{k}$

$i\omega_n \to \omega + i\eta$

$$\begin{cases} \omega = -\mu & \text{proportion } 1 - \langle n_{-\sigma}\rangle \text{ du temps} \\ \omega = -\mu + U & \text{'' } \langle n_{-\sigma}\rangle \text{ du temps} \end{cases}$$

Cas particulier $\mu = \frac{U}{2}$ $\langle n_{-\sigma}\rangle = \frac{1}{2}$

$$\mathcal{G}_\sigma(i\omega_n) = \frac{\frac{1}{2}}{i\omega_n + \frac{U}{2}} + \frac{\frac{1}{2}}{i\omega_n - \frac{U}{2}} = \left[\frac{i\omega_n}{(i\omega_n)^2 - \frac{U^2}{4}}\right]$$

$$= \frac{1}{i\omega_n - \frac{U^2}{4 i\omega_n}}$$

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

46: Hubbard dans les traces du gaz d'électrons

1. Prop. 1 particule

$$\ln Z[\varphi] = \ln \mathrm{Tr}\left[e^{-\beta K}\, T_\tau\, e^{-\psi^\dagger_{\bar\sigma}(\bar 1)\,\varphi_{\bar\sigma}(\bar 1,\bar 2)\,\psi_{\bar\sigma}(\bar 2)}\right]$$

$$\mathcal{G}_\sigma(1,2) = -\frac{\delta \ln Z}{\delta\varphi_\sigma(2,1)}$$

$$\boxed{\left(\mathcal{G}_{0\sigma}^{-1} - \varphi_\sigma - \Sigma_\sigma\right)\mathcal{G}_\sigma = 1}$$

$$\mathcal{G}_\sigma^{0\,-1}\,\mathcal{G}_\sigma = 1 + \Sigma_\sigma \mathcal{G}_\sigma + \varphi_\sigma \mathcal{G}_\sigma$$

$$\boxed{\mathcal{G}_\sigma^{-1} = \mathcal{G}_{0\sigma}^{-1} - \varphi_\sigma - \Sigma_\sigma}$$

$$\boxed{\Sigma_\sigma(1,\bar 1)\,\mathcal{G}_\sigma(\bar 1,2) = -U\left\langle \psi^\dagger_{-\sigma}(1)\,\psi_{-\sigma}(1)\,\psi_\sigma(1)\,\psi^\dagger_\sigma(2)\right\rangle}$$

$$= -U\left[\frac{\delta\mathcal{G}_\sigma(1,2)_\varphi}{\delta\varphi_{-\sigma}(1^+,1)} - \underline{\mathcal{G}_\sigma(1,2)_\varphi\,\mathcal{G}_{-\sigma}(1,1^+)_\varphi}\right]$$

$$\left[U\psi^\dagger_{-\sigma}\psi_{-\sigma}\psi_\sigma\cancel{\psi_\sigma},\ \cancel{\psi^\dagger_\sigma}\right]$$

$$\mathcal{G}_\sigma(1,2)_\varphi = -\left\langle T_\tau\, \psi(1)\,\psi^\dagger(2)\right\rangle \quad e^{\cdots}$$

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46.2 Fonctions de réponse.

$$\mathcal{G}_\sigma^{-1}\mathcal{G}_\sigma = 1 \qquad \frac{\delta \mathcal{G}_\sigma^{-1}}{\delta \varphi_{\sigma'}}\mathcal{G}_\sigma + \mathcal{G}_\sigma^{-1}\frac{\delta \mathcal{G}_\sigma}{\delta \varphi_{\sigma'}} = 0$$

$$\frac{\delta \mathcal{G}_\sigma}{\delta \varphi_{\sigma'}} = -\mathcal{G}_\sigma \frac{\delta \mathcal{G}_\sigma^{-1}}{\delta \varphi_{\sigma'}}\mathcal{G}_\sigma$$

$$\boxed{\frac{\delta \mathcal{G}_\sigma}{\delta \varphi_{\sigma'}} = \mathcal{G}_\sigma \frac{\delta \varphi_\sigma}{\delta \varphi_{\sigma'}}\mathcal{G}_\sigma + \mathcal{G}_\sigma \frac{\delta \Sigma_\sigma}{\delta \mathcal{G}_\sigma}\frac{\delta \mathcal{G}_\sigma}{\delta \varphi_{\sigma'}}\mathcal{G}_\sigma}$$

$$\frac{\delta \mathcal{G}_\sigma(1,1^+)_\varphi}{\delta \varphi_{\sigma'}(2^+,2)} = -\langle T_\tau \psi_\sigma^+(1^+)\psi_\sigma(1)\,\psi_{\sigma'}^+(2^+)\psi_{\sigma'}(2)\rangle_\varphi + \langle T_\tau \psi_\sigma^+(1^+)\psi_\sigma(1)\rangle_\varphi\langle T_\tau \psi_{\sigma'}^+(2^+)\psi_{\sigma'}(2)\rangle_\varphi$$

$$-\sum_{\sigma\sigma'}\frac{\delta \mathcal{G}_\sigma(1,1^+)}{\delta \varphi_{\sigma'}(2^+,2)} = \langle T_\tau n(1)\,n(2)\rangle_\varphi - \langle n(1)\rangle_\varphi\langle n(2)\rangle_\varphi$$

$$-\sum_{\sigma\sigma'}\sigma\frac{\delta \mathcal{G}_\sigma(1,1^+)}{\delta \varphi_{\sigma'}(2^+,2)}\sigma' = \langle T_\tau S^z(1)\,S^z(2)\rangle_\varphi - \langle S^z(1)\rangle_\varphi\langle S^z(2)\rangle_\varphi$$

$$-\sum_{\sigma\sigma'} \sigma \frac{\delta G_\sigma}{\delta \varphi_{\sigma'}} \sigma' = -2 G_\wedge G - \sum_{\sigma\sigma'} \sum_{\sigma''} G \, \boxed{\sigma \frac{\delta \Sigma_\sigma}{\delta G_{\sigma''}} \sigma''} \, \sigma'' \frac{\delta G_{\sigma''}}{\delta \varphi_{\sigma'}} \sigma' G$$

$$\sum_\sigma \frac{\delta \Sigma_\sigma}{\delta G_{\sigma''}} = \frac{\delta \Sigma_\uparrow}{\delta G_{\sigma''}} + \frac{\delta \Sigma_\downarrow}{\delta G_{\sigma''}}$$

$$\left(-\sum_{\sigma\sigma'} \frac{\delta G_\sigma}{\delta \varphi_{\sigma'}} \right) = -2 G_\wedge G + G \left[\left(\frac{\delta \Sigma_\uparrow}{\delta G_\uparrow} + \frac{\delta \Sigma_\uparrow}{\delta G_\downarrow} \right) \sum_{\sigma\sigma''} \frac{\delta G_{\sigma''}}{\delta \varphi_{\sigma'}} \right] G$$

$$\left(\cdot \sum_{\sigma\sigma'} \sigma \frac{\delta G_\sigma}{\delta \varphi_{\sigma'}} \sigma' \right) = -2 G_\wedge G - G \left[\frac{\delta \Sigma_\uparrow}{\delta G_\downarrow} - \frac{\delta \Sigma_\uparrow}{\delta G_\uparrow} \right] \sum_{\sigma\sigma''} \sigma'' \frac{\delta G_{\sigma''}}{\delta \varphi_{\sigma'}} \sigma'] G$$

$$\sum_\sigma \sigma \frac{\delta \Sigma_\sigma}{\delta G_{\sigma''}} \sigma'' = \frac{\delta \Sigma_\uparrow}{\delta G_{\sigma''}} \sigma'' - \frac{\delta \Sigma_\downarrow}{\delta G_{\sigma''}} \sigma''$$

$$= \frac{\delta \Sigma_\uparrow}{\delta G_\uparrow} - \frac{\delta \Sigma_\downarrow}{\delta G_\uparrow} = -\frac{\delta \Sigma_\uparrow}{\delta G_\downarrow} + \frac{\delta \Sigma_\downarrow}{\delta G_\downarrow}$$

$$\chi_{ch}(q) = \frac{\chi_0(q)}{1 + \frac{U}{2}\chi_0(q)}$$

$$\chi_{sp}(q) = \frac{\chi_0(q)}{1 - \frac{U}{2}\chi_0(q)}$$

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