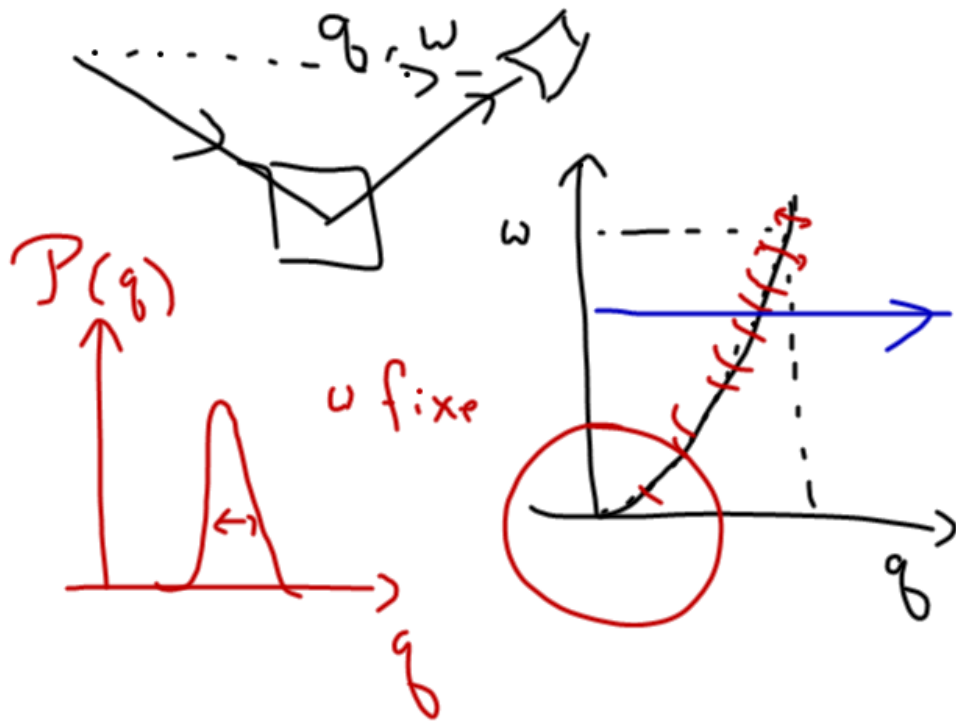


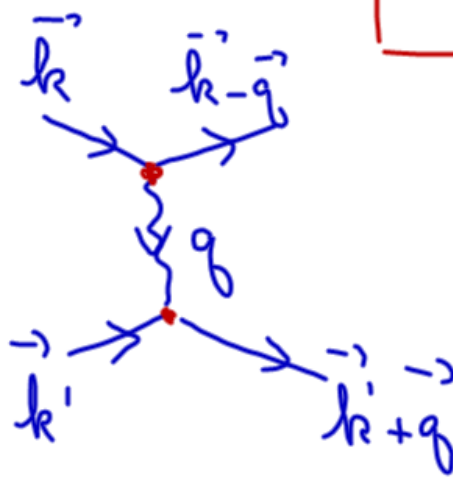
À venir



Meilleurs états à 1 particule  
(Approx. de Hartree-Fock)

$$H = \sum_{\sigma} \int d^3r \Psi_{\sigma}^{\dagger}(\vec{r}) \left( -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right) \Psi_{\sigma}(\vec{r})$$

$$+ \frac{1}{2} \sum_{\sigma\sigma'} \int d^3r d^3r' U(\vec{r}-\vec{r}') \Psi_{\sigma}^{\dagger}(\vec{r}) \Psi_{\sigma'}^{\dagger}(\vec{r}') \Psi_{\sigma'}(\vec{r}') \Psi_{\sigma}(\vec{r})$$



$$|\Phi_0\rangle = a_1^\dagger a_2^\dagger \dots a_n^\dagger |0\rangle$$

$$\rightarrow \Psi^+(\vec{r}) = \sum_n a_n^\dagger \varphi_n^*(\vec{r})$$

$$\rightarrow \Psi(\vec{r}) = \sum_n a_n \varphi_n(\vec{r})$$

Minimiser:

$$\langle \Phi_0 | H | \Phi_0 \rangle$$

$$\rightarrow \int \Psi^* \mathcal{D} \Psi d^3r = \sum_n E_n a_n^\dagger a_n \quad (a_1^\dagger, a_2^\dagger, a_3^\dagger, \dots |0\rangle)$$

Contrainte

$$\int d^3r \varphi_n^*(\vec{r}) \varphi_m(\vec{r}) = \delta_{nm}$$

Lemme:

$$\langle \Phi_0 | a_1^\dagger a_2 | \Phi_0 \rangle$$

$$\langle 0 | a_2 a_1^\dagger | 0 \rangle = 0$$

$$\langle 0 | a_1 a_1^\dagger | 0 \rangle = 1$$

$$\langle 0 | a_1 a_2 a_3^\dagger a_1^\dagger | 0 \rangle = 0$$

$$\langle \Phi_0 | a_i^+ a_j | \Phi_0 \rangle = \delta_{ij} \text{ si } i \text{ et } j \text{ occupés dans } |\Phi_0\rangle$$

$$\langle \Phi_0 | a_i^+ a_j^+ a_l a_l | \Phi_0 \rangle$$

Diagram showing the contraction of operators in the expectation value. Blue lines connect  $a_i^+$  to  $a_l$  and  $a_j^+$  to  $a_l$ . A box labeled  $l \neq k$  has an arrow pointing to the  $a_l$  operator. A box labeled  $j=k$  is under the  $a_l$  operator. A box labeled  $i=l$  is under the  $a_l$  operator.

$$a_j^+ a_l = -a_l a_j^+ \text{ si } l \neq j$$

$$= \delta_{il} \delta_{jk} - \delta_{ik} \delta_{jl}$$

Diagram showing the contraction of operators in the expectation value. Blue lines connect  $a_i^+$  to  $a_l$  and  $a_j^+$  to  $a_l$ . Red lines connect  $a_i^+$  to  $a_l$  and  $a_j^+$  to  $a_l$ .

$k=l$   
Théorème  
de Wick

Si  $i$  et  $j$  sont un des  
états de  $|\Phi_0\rangle$

$$a_3^+ a_1 \left[ c_0 (a_1^+ a_2^+ |0\rangle) + c_1 (a_3^+ a_2^+ |0\rangle) \right]$$

$$\left[ \langle 0 | a_2 a_1 c_0^* + \langle 0 | a_2 a_3 c_1^* \right]$$

The image shows a handwritten mathematical derivation. The top expression is  $a_3^+ a_1 [c_0 (a_1^+ a_2^+ |0\rangle) + c_1 (a_3^+ a_2^+ |0\rangle)]$ . The bottom expression is  $[\langle 0 | a_2 a_1 c_0^* + \langle 0 | a_2 a_3 c_1^*]$ . Red arrows indicate the contraction of operators: one arrow points from  $a_1^+$  in the top expression to  $a_1$  in the bottom expression; another points from  $a_2^+$  in the top expression to  $a_2$  in the bottom expression; a third points from  $a_3^+$  in the top expression to  $a_3$  in the bottom expression. A fourth arrow points from the  $a_1$  in the top expression to the  $a_1$  in the bottom expression.

$$\langle \Phi_0 | \int d^3r \psi^\dagger(\vec{r}) \mathcal{D} \psi(\vec{r}) | \Phi_0 \rangle$$

$$= \sum_{ij} \langle \Phi_0 | \int d^3r \varphi_i^*(\vec{r}) a_i^\dagger \mathcal{D} a_j \varphi_j(\vec{r}) | \Phi_0 \rangle$$

$$= \sum_{i=1}^N \int d^3r \varphi_i^*(\vec{r}) \mathcal{D} \varphi_i(\vec{r})$$

$$a_1 \dots a_n |0\rangle \equiv |\Phi_0\rangle$$

$$S: \text{pas } \langle \Phi_0 | \Phi_0 \rangle$$

$$\sum_{ij} a_i^\dagger a_j \int d^3r \varphi_i^*(\vec{r}) \mathcal{D} \varphi_j(\vec{r})$$

$t_{ij}$

$$\langle \Phi_0 | \frac{1}{2} \int d^3r d^3r' U(\vec{r} - \vec{r}')$$

$$\sum_{ijkl} \left[ \varphi_i^*(\vec{r}) a_i^\dagger \varphi_j^*(\vec{r}') a_j^\dagger \right] a_{h\sigma'} \varphi_h(\vec{r}') a_{l\sigma} \varphi_l(\vec{r}) | \Phi_0 \rangle$$

$$= \frac{1}{2} \int d^3r d^3r' U(\vec{r} - \vec{r}') \sum_{ij} |\varphi_i(\vec{r})|^2 |\varphi_j(\vec{r}')|^2$$

$$- \frac{1}{2} \int d^3r d^3r' U(\vec{r} - \vec{r}') \sum_{ij} \varphi_i^*(\vec{r}) \varphi_i(\vec{r}') \varphi_j^*(\vec{r}') \varphi_j(\vec{r})$$

Échange = Fock

$$\varphi_j^*(\vec{r}') \varphi_j(\vec{r})$$

$$\left\{ \frac{\partial}{\partial \varphi_i^*(\vec{r})} \left[ \langle \Phi_0 | H | \Phi_0 \rangle + \sum_{ij} \gamma_{ij} \int d^3r \varphi_i^*(\vec{r}) \varphi_j(\vec{r}) \right] = 0 \right.$$

$$\left. \sum_i (-\epsilon_i) \int d^3r \varphi_i^*(\vec{r}) \varphi_i(\vec{r}) \right.$$

$$f(x, y)$$

Contrainte

$$\frac{\partial f}{\partial x} = 0$$

$$\frac{\partial f}{\partial y} = 0$$

$$g(x, y) = 0$$

Lagrange

$$y(x) \rightarrow \frac{\partial f(x, y(x))}{\partial x} = 0$$

$$dg = 0 \quad dy = \frac{\partial g}{\partial x} dx + \frac{\partial g}{\partial y} dy = 0$$

$$df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy = 0$$

$$df + \lambda dg = 0$$

$$\left( \frac{\partial f}{\partial x} + \lambda \frac{\partial g}{\partial x} \right) dx + \left( \frac{\partial f}{\partial y} + \lambda \frac{\partial g}{\partial y} \right) dy = 0$$

$$\downarrow$$

$$0$$

$$\downarrow$$

$$0$$

$$f(x(\lambda), y(\lambda))$$

$$g(x(\lambda), y(\lambda)) = 0$$



Terme à 1 corps:

$$\mathcal{D} \varphi_i(\vec{r}''') - \epsilon_i \varphi_i(\vec{r}''')$$

$$+ \int d^3 r' U(\vec{r}'' - \vec{r}') \varphi_i(\vec{r}''') \sum_j |\varphi_j(\vec{r}')|^2$$

$$- \int d^3 r' U(\vec{r}'' - \vec{r}') \varphi_i(\vec{r}') \underbrace{\sum_j}_{\rho(\vec{r}')}$$

$$\sum_j \varphi_j^*(\vec{r}') \varphi_j(\vec{r}') = 0$$

$$\left[ \mathcal{D} \varphi_i(\vec{r}) + \int d^3 r' U(\vec{r} - \vec{r}') \rho(\vec{r}') \right] \varphi_i(\vec{r})$$

$$- \int d^3 r' U(\vec{r} - \vec{r}') \sum_j \varphi_j^*(\vec{r}') \varphi_j(\vec{r}') \varphi_i(\vec{r}') \right]$$

$$= \epsilon_i \varphi_i(\vec{r})$$

$$\mathcal{D} \varphi_i(\vec{r}) + U_H(\vec{r}) \varphi_i(\vec{r})$$

$$- \int d^3 r' \underbrace{V_E(\vec{r}, \vec{r}')}_{\text{Non local}} \varphi_i(\vec{r}') = \epsilon_i \varphi_i(\vec{r})$$

Non local

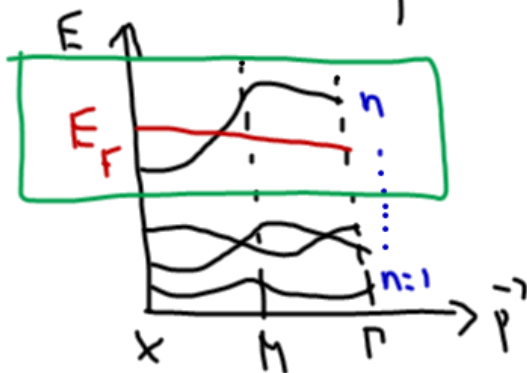
$$|\Phi_0\rangle = a_1^\dagger a_2^\dagger \dots a_n^\dagger |\Phi_0\rangle$$

# Bandes étroites "d"

s, p Bandes + perturbations

① Théorie des bandes

② 
$$\Psi^+(\mathbf{r}) = \sum_{n, \vec{p}} \varphi_{n, \vec{p}}^*(\vec{r}) a_{n, \vec{p}}^+$$



$$\varphi_{n, \vec{p}}(\vec{r}) = e^{i\vec{p} \cdot \vec{r}} u_n(\vec{r})$$

$$u_n(\vec{r} + \vec{R}) = u_n(\vec{r})$$

③ Une seule bande

④ États de Wannier

$$W_n(\vec{r} - \vec{R}) = \sqrt{V_P} \int \frac{d^3 p}{(2\pi)^3} e^{-i\vec{p} \cdot \vec{R}} \varphi_{n, \vec{p}}(\vec{r})$$

$$= \sqrt{V_P} \int \frac{d^3 p}{(2\pi)^3} e^{i\vec{p} \cdot (\vec{r} - \vec{R})} u_n(\vec{r})$$

Dans la base de Wannier

$$\sum_{\sigma} \sum_{ij} \langle i\sigma | D | j\sigma \rangle c_i^{\dagger} c_j$$

où  $c_i^{\dagger}$  crée une ptcle

dans l'état de Wannier  $W(\vec{r} - \vec{R}_i)$

$$\sum_{ij} t_{ij} c_i^{\dagger} c_j$$

laisse tomber  
 $n$

$$t_{ij} = \langle i\sigma | D | j\sigma \rangle$$

Terme à 2 corps:

$$\frac{1}{2} \sum_{ijkl} \langle i\sigma | \langle j\sigma' | V(\vec{r}-\vec{r}') | l\sigma \rangle | k\sigma' \rangle$$

$$c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{l\sigma} c_{k\sigma'}$$

$$\langle i\sigma | \langle j\sigma' | V(\vec{r}-\vec{r}') | l\sigma \rangle | k\sigma' \rangle$$

$$= \int d^3r d^3r' V(\vec{r}-\vec{r}') w^*(\vec{r}-\vec{R}_i) w^*(\vec{r}'-\vec{R}_j)$$

$$w(\vec{r}-\vec{R}_l) w(\vec{r}'-\vec{R}_k)$$

Hubbard

Élément de matrice max. lorsque  
 $i=j=k=l$

H à 2 corps devient:

$$\frac{1}{2} \sum_{i\sigma} U c_{i\sigma}^\dagger c_{i\sigma}^\dagger c_{i\sigma} c_{i\sigma}$$

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

$$= \frac{1}{2} \sum_{i\sigma} U n_{i\sigma} n_{i-\sigma}$$

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

$$U = \int d^3r d^3r' V(\vec{r}-\vec{r}') |w(\vec{r})|^2 |w(\vec{r}')|^2$$

Hamiltonien de Hubbard

$$H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$\sum_{k\sigma} e^{ik\cdot R_i} c_{k\sigma}^\dagger c_{k\sigma}$$

$$c_{k\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_{i=1}^N e^{-ik\cdot R_i} c_{i\sigma}^\dagger$$

$$\sum_i U_{n_i \uparrow n_i \downarrow} \left[ c_{1\uparrow}^+ c_{2\downarrow}^+ c_{3\uparrow}^+ \dots |0\rangle \right]$$

$N \uparrow \uparrow \downarrow \uparrow \downarrow \uparrow$

$2^N$  états fondamentaux  
 $\downarrow \downarrow \downarrow \uparrow \downarrow \uparrow$

$$- \uparrow \downarrow \uparrow \downarrow U \quad E=0$$

$$U - \uparrow \downarrow \uparrow \downarrow$$

Diagonalise  $t$   
 $\rightarrow c_{h_1\uparrow}^+ c_{h_2\downarrow}^+ \dots \sum_i c_i^+ e^{-i h_i \mathcal{R}_i} c_{h_n\uparrow}^+ c_{h_n\downarrow}^+ |0\rangle$

Diagonalise  $U$   
 $\rightarrow c_{1\uparrow}^+ c_{2\downarrow}^+ \dots c_{N\uparrow}^+ |0\rangle$

Limite  $U \gg t$  "localisés"  
 $n=1$

Transition de Mott