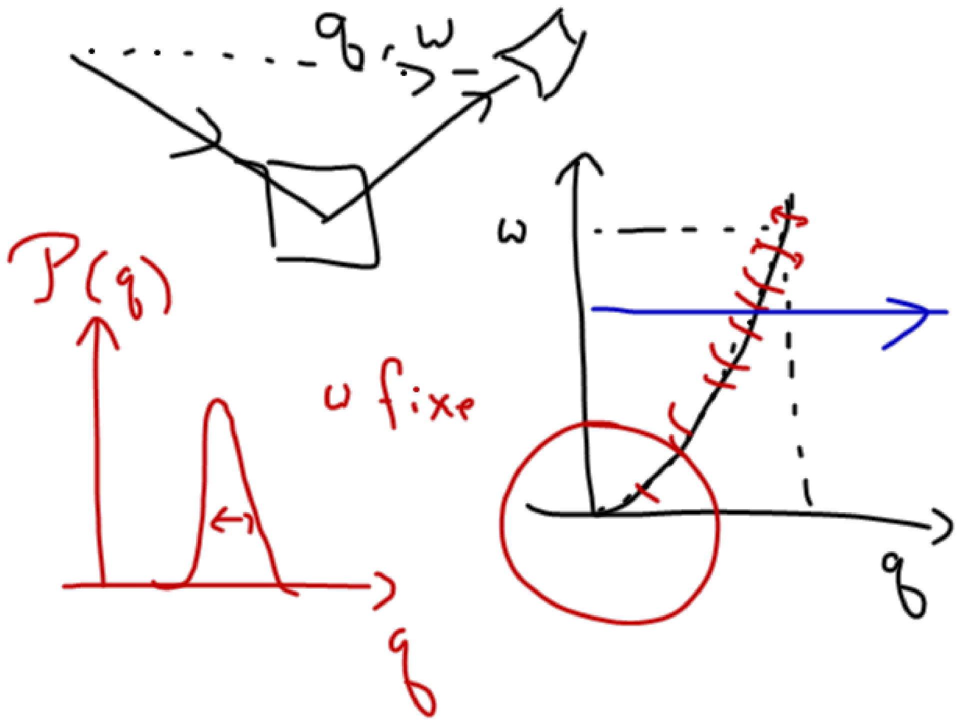
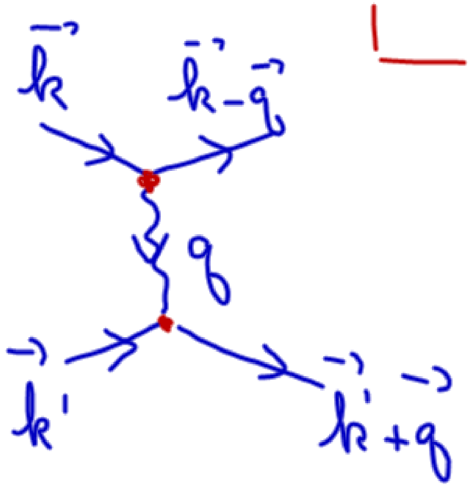
À venir



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

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

$$+ \frac{1}{2} \sum_{\sigma\sigma'} \int d^3r \, d^3r' \; U(\vec{r}-\vec{r}\,') \, \psi^{\dagger}_{\sigma}(\vec{r}) \, \psi^{\dagger}_{\sigma'}(\vec{r}\,') \, \psi_{\sigma'}(\vec{r}\,') \, \psi_{\sigma}(\vec{r})$$



$$\boxed{|\Phi_0\rangle = a_1^\dagger a_2^\dagger \dots a_N^\dagger |0\rangle}$$

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

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

Minimiser :

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

Contrainte

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

$$\rightarrow \int \psi^\dagger D \psi \, d^3r$$

$$= \sum_n E_n a_n^\dagger a_n \quad (a_1^\dagger a_2^\dagger a_3^\dagger)|0\rangle$$

Lemme :

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

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

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

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

$$\langle \Phi_0 | a_i^+ a_j | \Phi_0 \rangle = \delta_{ij}$$

si i et j occupés dans $|\Phi_0\rangle$

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

$\boxed{l \neq k}$

$j = k$

$i = l$

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

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

$k = l$

Théorème de Wick

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

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

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

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

$$= \sum_{ij} \langle \Phi_0 | \int d^3r \, \varphi^*_i(r) \, a^\dagger_i \, D \, a_j \, \varphi_j(\vec r) \, | \Phi_0 \rangle$$

$$= \boxed{\sum_{i=1}^{N} \int d^3r \, \varphi^*_i(r) \, D \, \varphi_i(r)} \qquad D^2_{\vec r} \, \varphi$$

$$a_1 \dots a_N |0\rangle = |\Phi_0\rangle$$

Si pas $\langle \Phi_0 |$ $| \Phi_0 \rangle$

$$\sum_{ij} a^\dagger_i a_j \underbrace{\boxed{\int d^3r \, \varphi^*_i(\vec r) \, D \, \varphi_j(r)}}_{t_{ij}}$$

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

$$\sum_{ijkl} \varphi^*_i(\vec{r}\,)\, a^+_{i\sigma}\, \varphi^*_j(\vec{r}\,')\, a^+_{j\sigma'}\, a_{k\sigma'}\, \varphi_k(\vec{r}\,')\, a_{l\sigma}\, \varphi_l(\vec{r}\,) |\Phi_0\rangle$$

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

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

Échange ≡ Fock

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

$$\sum_i (-\epsilon_i) \int d^3r \, \varphi_i^*(r) \varphi_i(r)$$

$$\boxed{f(x,y)} \qquad \frac{\partial f}{\partial x} = 0 \quad \frac{\partial f}{\partial y} = 0$$

Contrainte

$$\boxed{g(x,y) = 0}$$

Lagrange

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

$$dg = 0$$

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

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

$$df + \lambda \, dg = 0$$

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

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

$$\boxed{g\big(x(\lambda), y(\lambda)\big) = 0}$$

Terme à 1 corps :

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

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

$$-\int d^3r'\, U(\vec{r}''-\vec{r}')\,\varphi_i(r')\sum_j \varphi_j^*(\vec{r}')\,\varphi_j(\vec{r}'') = 0$$

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

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

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

$$\boxed{\begin{aligned}&\mathcal{D}\,\varphi_i(\vec{r}) + U_H(\vec{r})\,\varphi_i(\vec{r})\\ &\quad - \int d^3r'\,\underbrace{V_E(\vec{r},\vec{r}')}_{\text{Non local}}\,\varphi_i(\vec{r}') = \epsilon_i\,\varphi_i(\vec{r})\end{aligned}}$$

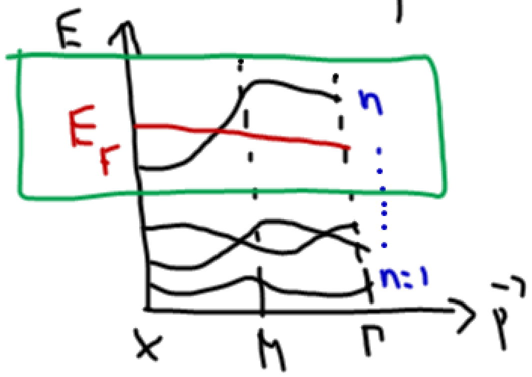
$$|\Phi_0\rangle = a_1^+ a_2^+ \dots a_N^+ |\Phi_0\rangle$$

Bandes étroites "d"

s, p Bandes + perturbations

① Théorie des bandes

② $\Psi^+(r) = \sum_{n,\vec{p}} \varphi^*_{n,\vec{p}}(\vec{r})\, a^+_{n,\vec{p}}$



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

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

③ Une seule bande

④ États de Wannier

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

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

Dans la base de Wannier

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

où c_i^+ crée une ptcle dans l'état de Wannier $w(\vec{r}-\vec{R}_i)$

laisse tomber n

$$\sum_{ij\sigma} t_{ij} c_i^+ c_j$$

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

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Terme à 2 corps :

$$\frac{1}{2}\sum_{\substack{ijkl\\ \sigma\sigma'}} \langle i\sigma| \langle j\sigma'| V(\vec{r}-\vec{r}\,') |k\sigma\rangle |l\sigma'\rangle \; c^{+}_{i\sigma} c^{+}_{j\sigma'} c_{l\sigma'} c_{k\sigma}$$

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

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

Hubbard

Elément de matrice max. lorsque

$$i=j=k=l$$

H à 2 corps devient :

$$\frac{1}{2}\sum_{\substack{i\\ \sigma\sigma'}} U\, c^{+}_{i\sigma} c^{+}_{i\sigma'} c_{i\sigma'} c_{i\sigma}$$

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

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

$$= \sum_{i} U\, n_{i\uparrow} n_{i\downarrow}$$

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

Hamiltonien de Hubbard

$$H = \underbrace{\sum_{ij\sigma} t_{ij}\, c^{+}_{i\sigma} c_{j\sigma}}_{\to\, 0} + \underbrace{U \sum_{i} n_{i\uparrow} n_{i\downarrow}}_{\to\, 0}$$

$$\sum_{k\sigma} \epsilon(k)\, c^{+}_{k\sigma} c_{k\sigma}$$

$$c^{+}_{k\sigma} = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} e^{-i\vec{k}\cdot\vec{R}_i}\, c^{+}_{i\sigma}$$

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$$\sum_i U\, n_{i\uparrow} n_{i\downarrow} \left[c^+_{1\uparrow} c^+_{2\downarrow} c^+_{3\uparrow} \dots |0\rangle \right]$$

N ↑ ↑ ↓ ↑ ↓ ↑

↓ ↓ ↓ ↑ ↓ ↑

2^N états fondamentaux

$-$ ↑↓ t ↑ ↓ U $E=0$

U $-$ ↑↓ t ↑ ↓

Diagonalise t $\quad \sum_i c^+_i e^{-ik_q \cdot R_i}$

$$\longrightarrow \underbrace{c^+_{k_0\uparrow} c^+_{k_0\downarrow} \dots c^+_{k_n\uparrow}} c^+_{k_n\downarrow} |0\rangle$$

Diagonalise U

$$\longrightarrow \underbrace{c^+_{1\uparrow} c^+_{2\downarrow} \dots c^+_{N\uparrow}} |0\rangle$$

Limite $\boxed{U \gg t \quad \text{"localisés"} \quad n = 1}$

Transition de Mott