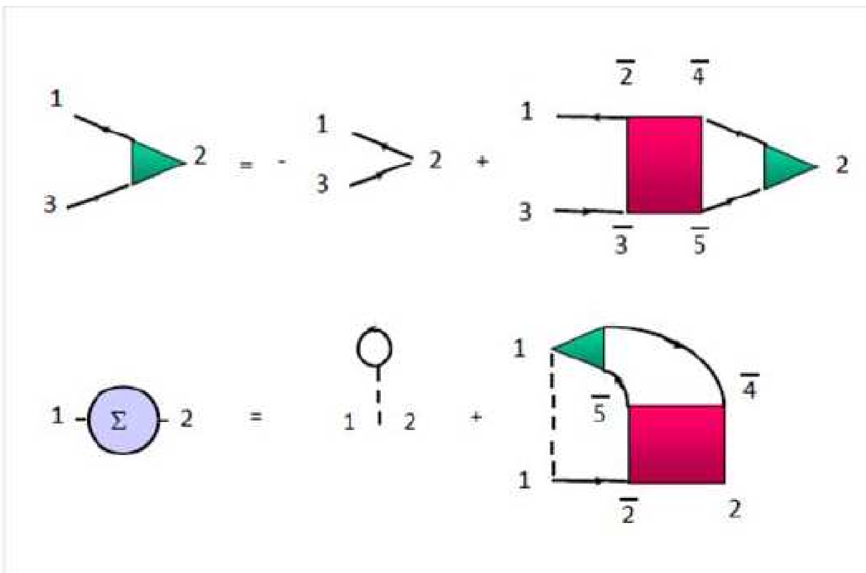
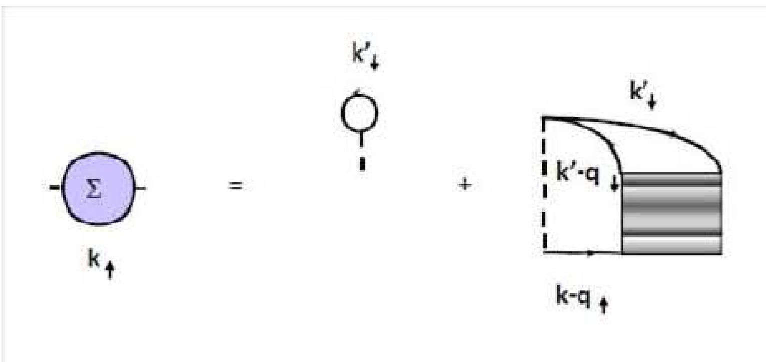


1
2
3
=
-
1
2
3
+
$\bar{2}$
$\bar{4}$
1
2
3
$\bar{3}$
$\bar{5}$
1
Σ
2
=
1
2
+
1
$\bar{5}$
$\bar{4}$
1
$\bar{2}$
2



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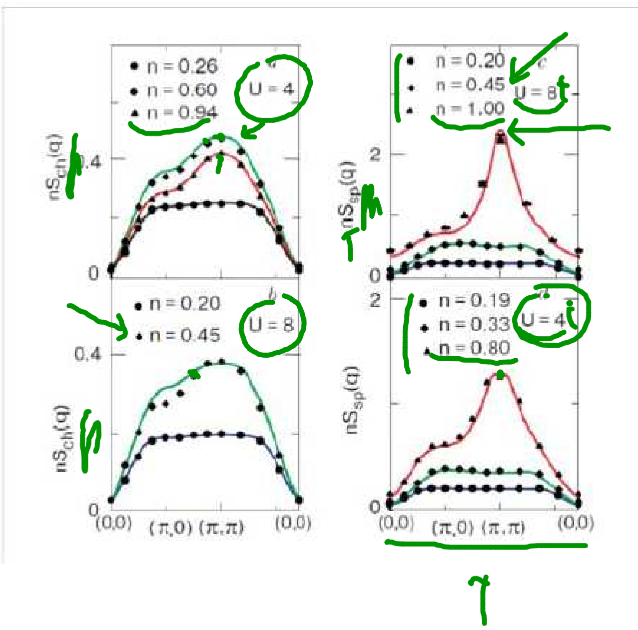
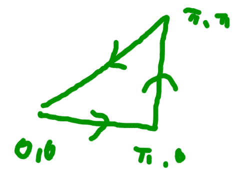


n = 0.26
n = 0.60
n = 0.94
U = 4
nSch(q)
0.4
0
n = 0.20
n = 0.45
n = 1.00
U = 8
nSsp(q)
2
0
n = 0.20
n = 0.45
U = 8
0.4
nSch(q)
0
(0,0) (π,0) (π,π) (0,0)
2
n = 0.19
n = 0.33
n = 0.80
U = 4
nSsp(q)
0
(0,0) (π,0) (π,π) (0,0)
q

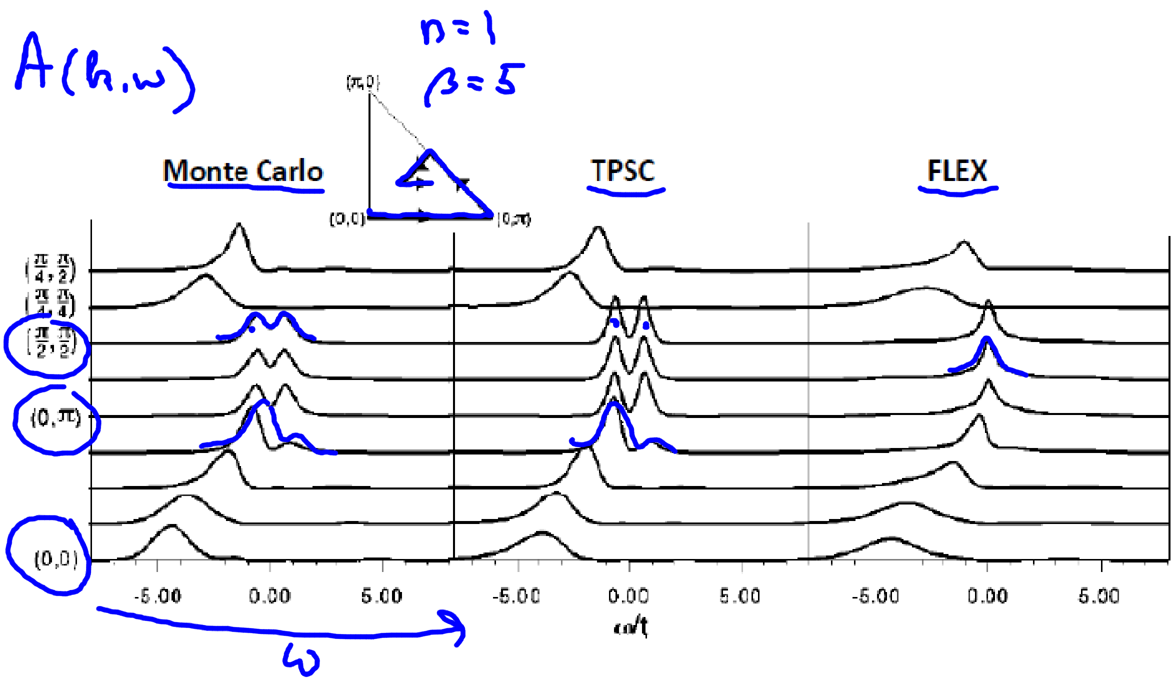
$\beta = 5$

$T = 0.2t$



π,π
0,0
π,0

$A(k,\omega)$



n=1
β=5
Monte Carlo
TPSC
FLEX
(π,0)
(0,0)
(0,π)
(π/4, π/2)
(π/4, π/4)
(π/2, π/2)
(0,π)
(0,0)
-5.00
0.00
5.00
ω/t
ω

46.3 Hartree-Fock + RPA ✓
46.4 RPA et principe de Pauli: ✓
46.5 RPA transition de phase et Mermin-Wagner ✓

47. Approche Auto-Cohérente à deux particules ACDP-TPSC
47.1 Étape 1. Modes collectifs, auto-cohérence à 2 particules
47.2 Étape 2. Meilleure self-énergie
47.3 Test de précision - Cohérence 1 et 2 particules

48. TPSC test de précision, aspects physiques ✓

48.1 Approche physique, spin et charge ✓

48.2 Mermin-Wagner, Kanamori-Brueckner ✓

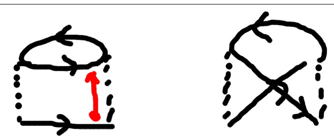
48.3 Comparaisons

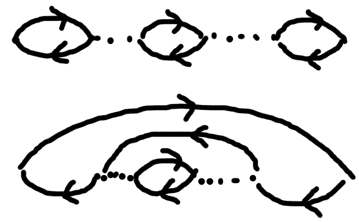
1. Spin-charge ✓
2. Self ✓

48.4 Pseudogap ?

49. Théorie de champ moyen dynamique DMFT

49.1 Impuretés quantiques





$U = 0$

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

$$\left.\begin{array}{l}\epsilon_k^{max} = 4t \\ \epsilon_k^{min} = -4t\end{array}\right\} W = 8t$$

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46.3 H.F. + RPA

$$\frac{\delta \mathcal{G}}{\delta \phi} = \mathcal{G}\,\mathcal{G} + \mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right)\mathcal{G}$$

$$\chi_{ch}(1,2) = -\sum_{\sigma\sigma'} \frac{\delta\mathcal{G}_\sigma(1,1^+)}{\delta\phi_{\sigma'}(2^+,2)} = -2\,\mathcal{G}(1,2)\,\mathcal{G}(2,1)$$

$$-\mathcal{G}(1,\bar3)\overbrace{\left(\frac{\delta\Sigma_\uparrow(\bar3,\bar4)}{\delta\mathcal{G}_\uparrow(\bar6,\bar7)} \pm \underbrace{\frac{\delta\Sigma_\uparrow(\bar3,\bar4)}{\delta\mathcal{G}_\downarrow(\bar6,\bar7)}}_{-U_{sp}}\right)}^{U_{ch}}\sum_{\sigma\sigma'}\frac{\delta\mathcal{G}_{\sigma}(\bar6,\bar7)}{\delta\phi_{\sigma'}(2^+,2)}\,\mathcal{G}(\bar4,1^+)$$

Calcul des pages suivantes

$$\chi_{ch}(1,2) = \overset{\chi_0}{\boxed{-2\,\mathcal{G}(1,2)\,\mathcal{G}(2,1)}} + \mathcal{G}(1,\bar3)\,\mathcal{G}(\bar3,1^+)\,U\,\chi_{ch}(\bar3,2)$$

$$\chi_{ch}(q) = \chi(q) - \frac{U}{2}\chi_0(q)\,\chi_{ch}(q)$$

$$\boxed{\chi_{\substack{ch\\sp}}(q) = \frac{\chi_0(q)}{1 \pm \frac{U}{2}\chi_0(q)}}$$

$$\Sigma_\sigma(1,\bar 1)\,\mathcal{G}_\sigma(\bar 1,2) = -i\,U\langle T_\tau\, \psi^+_{-\sigma}(1^+)\psi_{-\sigma}(1)\psi_\sigma(1)\psi^+_\sigma(2)\rangle$$

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

0

$$\mathcal{G}^{-1}_\varphi = \mathcal{G}_0^{-1} - \varphi_\varphi - \Sigma_\varphi$$

$$\mathcal{D}\mathcal{G} + \mathcal{G}\,\frac{\delta\Sigma}{\delta\varphi}\,\mathcal{G}$$

$$\frac{\delta\mathcal{G}}{\delta\varphi}\mathcal{G}^{-1} + \mathcal{G}\,\delta\frac{\mathcal{G}^{-1}}{\delta\varphi} = 0$$

$$\left[\Sigma_\sigma(1,\bar{1})_q \mathcal{G}_\sigma(\bar{1},\bar{2})_q = U\,\mathcal{G}_{-\sigma}(1,1^+)_q \mathcal{G}_\sigma(1,\bar{2})_q\right]\mathcal{G}^{-1}(\bar{2},3)$$

$$\Sigma_\sigma(1,3)_q = U\,\mathcal{G}_{-\sigma}(1,1^+)_q\,\delta(1-3)$$

$$\frac{\delta\Sigma_\sigma(1,3)}{\delta\mathcal{G}_{-\sigma}(4,5)} = \delta(1-3)\,U\,\delta(1-4)\,\delta(1^+-5) \qquad \frac{\delta\Sigma_\sigma}{\delta\mathcal{G}_\sigma} = 0$$

$$\rightarrow U_{sp}\,\delta(1-3)\,\delta(1-4)\,\delta(1-5^+) = U\,\delta(1-3)\,\delta(1-4)\,\delta(1^+-5)$$

46.4 RPA et principe de Pauli

$$\chi_{ch}(1,1) = \langle n(1)\, n(1)\rangle - \langle n(1)\rangle^2$$

$$= \langle (n_\uparrow + n_\downarrow)(n_\uparrow + n_\downarrow)\rangle - n^2$$

$$= \langle n_\uparrow^2\rangle + \langle n_\downarrow^2\rangle + 2\langle n_\uparrow n_\downarrow\rangle - n^2$$

$$= n + 2\langle n_\uparrow n_\downarrow\rangle - n^2$$

$$\chi_{sp}(1,1) = \langle (n_\uparrow - n_\downarrow)(n_\uparrow - n_\downarrow)\rangle = n - 2\langle n_\uparrow n_\downarrow\rangle$$

$$\boxed{\chi_{ch}(1,1) + \chi_{sp}(1,1) = 2n - n^2} \quad \text{indép. de } U$$

$$\frac{T}{N}\sum_{\vec{q}}\sum_{iq_n} e^{i\vec{q}\cdot(r_i - r_j) - iq_n(\tau_i - \tau_j)}\,\chi(\vec{q}, iq_n)$$

$$= \chi(r_i, \tau_i; r_j, \tau_j)$$

$$\boxed{\frac{T}{N}\sum_q (\chi_{ch} + \chi_{sp}) = 2n - n^2}$$

$$\frac{T}{N}\sum_q \left(\frac{\chi_0}{1 + \frac{U}{2}\chi_0} + \frac{\chi_0}{1 - \frac{U}{2}\chi_0}\right) = 2n - n^2$$

$$\chi_0(q) = \int \frac{d\omega}{\pi}\,\frac{\chi''(\omega)}{iq_n - \omega}$$

$$= \int \frac{d\omega}{\pi}\,\frac{\omega\,\chi''(\omega)}{q_n^2 + \omega^2}$$

46.5 Transitions de phase et Mermin-Wagner

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

$$\boxed{\chi_{sp}(\vec{q},0) \to \infty}$$

Cas particulier

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

Demi-rempli : $\mu = 0$

Soit

$$q = Q = (\pi,\pi,\pi)$$

$$\epsilon_{k+Q} = -\epsilon_k$$

$$\chi_0(q) = -2\sum_k \frac{f(\epsilon_k)-f(\epsilon_{k+q})}{\epsilon_k-\epsilon_{k+q}}$$

$$\chi_0(Q) = -2\sum_k \frac{2f(\epsilon_k)-1}{2\epsilon_k}$$

$$\boxed{f(-\epsilon_k) = 1-f(\epsilon_k) \qquad \frac{1}{e^{-\beta\epsilon_k}+1} = 1-\frac{1}{e^{\beta\epsilon_k}+1}}$$

$$= +2\sum_k \frac{\tanh(\beta\epsilon_k/2)}{2\epsilon_k}$$

$$= \int_{-\infty}^{\infty} d\epsilon\, N(\epsilon)\frac{\tanh(\beta\epsilon/2)}{2\epsilon} \sim 2N(0)\int_0^{\Lambda}\frac{\tanh\frac{\beta\epsilon}{2}}{2\epsilon}d\epsilon$$

$$\sim 2N(0)\int_T^{\Lambda}\frac{1}{2\epsilon}\,d\epsilon + \text{reg}$$

$$\sim 2N(0)\ln\frac{\Lambda}{T}$$

$$\boxed{1-\frac{U}{2}\,2N(0)\ln\frac{\Lambda}{T} = 0}$$

47. ACDP - TPSC

47.1 Etape 1

$$\frac{\delta \mathcal{G}_{-\sigma-\sigma}(1,2)}{\delta \varphi_{-\sigma\sigma}(1^+,1)}\Bigg|_{\varphi=0}$$

$$\Sigma_\sigma(1,\bar{1})_\varphi \mathcal{G}_\sigma(\bar{1},2)_\varphi = -U\langle T_\tau \psi^+_{-\sigma}(1^+)\psi_{-\sigma}(1)\psi_\sigma(1)\psi^+_\sigma(2)\rangle$$

imposé

$$\boxed{\Sigma_\sigma(1,\bar{1})_\varphi \mathcal{G}_\sigma(\bar{1},1^+)_\varphi = U\langle n_\downarrow n_\uparrow\rangle_\varphi}$$

$$\langle n_\uparrow n_\uparrow\rangle = \langle n_\uparrow\rangle$$

$$\boxed{\Sigma_\sigma(1,\bar{1})_\varphi \mathcal{G}_\sigma(\bar{1},2)_\varphi \doteq A_\varphi\, \mathcal{G}_{-\sigma}(1,1^+)_\varphi\, \mathcal{G}_\sigma(1,2)_\varphi}$$

$$U\langle n_\uparrow n_\downarrow\rangle_\varphi = A_\varphi \langle n_\downarrow\rangle_\varphi \langle n_\uparrow\rangle_\varphi$$

$$\boxed{A_\varphi = \frac{U\langle n_\uparrow n_\downarrow\rangle_\varphi}{\langle n_\uparrow\rangle_\varphi\langle n_\downarrow\rangle_\varphi}}$$

HF

$$\Sigma^{HF}_\sigma(1,3) = U\delta(1-3)\mathcal{G}_{-\sigma}(1,1^+)$$

$$\boxed{\Sigma^{TPSC}_\sigma(1,3)_\varphi = \frac{U\langle n_\uparrow n_\downarrow\rangle_\varphi}{\langle n_\uparrow\rangle_\varphi\langle n_\downarrow\rangle_\varphi}\,\mathcal{G}_{-\sigma}(1,1^+)_\varphi\,\delta(1-3)}$$

$$U_{sp} \to \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\downarrow} - \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\uparrow}$$

$$\boxed{U_{sp} = \frac{U\langle n_\uparrow n_\downarrow\rangle}{\langle n_\uparrow\rangle\langle n_\downarrow\rangle}}$$

U_{ch}

$$\frac{T}{N}\sum_q \chi_{sp} = \frac{T}{N}\sum_q \frac{\chi_0(q)}{1-\frac{U_{sp}}{2}\chi_0(q)} = n - 2\langle n_\uparrow n_\downarrow\rangle$$

$$\frac{T}{N}\sum_q \frac{\chi_0(q)}{1+\frac{U_{ch}}{2}\chi_0(q)} = n + 2\langle n_\uparrow n_\downarrow\rangle - n^2$$

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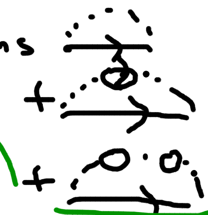
$$\chi_{ch}(q=0,\omega\neq 0)=0 \qquad \langle N(t)N(0)\rangle$$

Conservation $\qquad \to \delta(\omega)$

47.2 Etape 2

Gaz d'électrons



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

$$= U\mathcal{G}_{-\sigma}(1,1^+)\delta(1-2) - U\frac{\delta\mathcal{G}_\sigma(1,\bar{2})}{\delta\varphi_{-\sigma}(1^+,1)}\mathcal{G}_\sigma^{-1}(\bar{2},2)$$

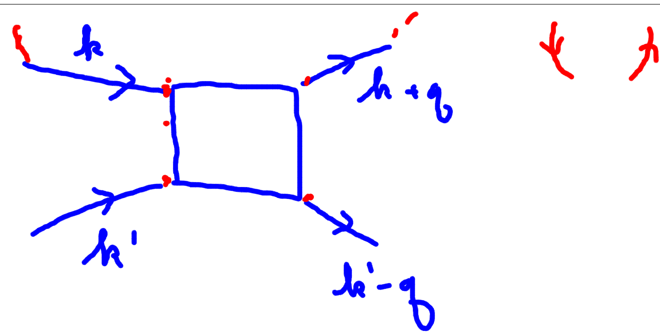
$$\frac{\delta\mathcal{G}}{\delta\varphi_{-\sigma}}\mathcal{G}_\sigma^{-1} = -\mathcal{G}_\sigma\frac{\delta\mathcal{G}_\sigma^{-1}}{\delta\varphi_{-\sigma}} \qquad \mathcal{G}^{-1}=\mathcal{G}_0^{-1}-\varphi-\Sigma$$

$$= +\mathcal{G}_\sigma\frac{\delta\Sigma_\sigma}{\delta\mathcal{G}_{\bar{\sigma}}}\frac{\delta\mathcal{G}_{\bar{\sigma}}}{\delta\varphi_{-\sigma}}$$

$$\Sigma^{(2)}(k) = Un_{-\sigma} + \frac{T}{N}\frac{U}{8}\sum_q\left[U_{sp}3\chi^{(1)}_{sp}(q)+U_{ch}\chi^{(1)}_{ch}(q)\right]\mathcal{G}^{(1)}_\sigma(k+q)$$

$$\Sigma(1,\bar{1})\mathcal{G}(\bar{1},1^+) = U\langle n_\uparrow n_\downarrow\rangle$$

$$\boxed{\frac{T}{N}\sum_k \Sigma^{(2)}(k)\,\mathcal{G}^{(1)}(k)\,e^{-ik_n0^-} = U\langle n_\uparrow n_\downarrow\rangle}$$


k
k + q
k'
k' - q

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