5.4 Prop. à 1 particule.

1. Hartree-Fock

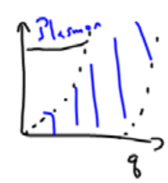
"Pathologies"

5.3 Formalisme.

1. Cohérence entre Σ et χ_{nn}
2. Énergie libre.

2. Guérison de H.-F.

Écrantage — Osc. plasma



$$r_s \propto \frac{1}{k_F a_0} \propto \frac{1}{(n_0 a_0)^{1/3}}$$

$$\nabla \cdot E = 4\pi \left[\rho_e + \langle \delta\rho \rangle \right]$$

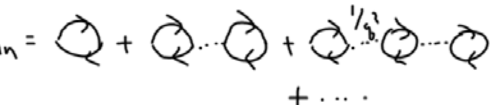
$$\epsilon_L \nabla \cdot E = 4\pi \rho_e \rightarrow \phi_e(q,\omega) = \frac{4\pi}{q^2} \rho_e(q,\omega)$$

$$\mathcal{H} = \int d^3r \, \rho(r) \, \phi_e(r)$$

$$\langle \delta\rho \rangle = -e^2 \chi_{nn}(q) \, \phi_e(\phi)$$

$$\epsilon_L^{-1} = \frac{\rho_e + \langle \delta\rho \rangle}{\rho_e} = 1 + \frac{\langle \delta\rho \rangle}{\rho_e}$$

$$\boxed{\frac{1}{\epsilon_L} = 1 - \frac{4\pi e^2}{q^2} \chi_{nn}(q,\omega)}$$

$\chi_{nn} =$ 

$$\chi_{nn} = \chi^0_{nn} - V_q \chi^0_{nn} \chi_{nn}$$

$$V_q \chi_{nn} = \frac{V_q \chi^0_{nn}}{1 + V_q \chi^0_{nn}} \rightarrow \frac{1}{1 + V_q \chi^0_{nn}(q,\omega)} = \frac{1}{\epsilon_L}$$

$$\boxed{\epsilon_L = 1 + V_q \chi^0_{nn}(q,\omega)}$$

$$\chi^0_{nn}(q,\omega) = -2 \int \frac{d^3k}{(2\pi)^3} \frac{f(\xi_k) - f(\xi_{k+q})}{\omega + \xi_k - \xi_{k+q}}$$

$\boxed{\omega = 0}$

$$q \to 0 \quad \chi^0_{nn}(q,0) = +2 \frac{\partial}{\partial\mu} \int \frac{d^3k}{(2\pi)^3} f(\xi_k)$$

$$= \frac{\partial n}{\partial \mu}$$

$$\boxed{\epsilon_L = 1 + \frac{q_{TF}^2}{q^2}} \qquad \frac{V_q}{\epsilon_L} = \frac{4\pi e^2}{q^2 \left(1 + \frac{q_{TF}^2}{q^2}\right)}$$

$$\omega \gg \xi_k - \xi_{k+q} \quad \forall \; k \text{ et } q$$

$$\epsilon^L(q \to 0, \omega) = 1 - \frac{\omega_p^2}{\omega^2} - \frac{3}{5} \frac{\omega_p^2}{\omega^2} \frac{(v_F q)^2}{\omega^2}$$

ω_p

$$\omega \sim \omega_p \quad (\omega - \omega_p)$$

$$\boxed{\epsilon^L(q \to 0, \omega) = 1 - \frac{\omega_q^2}{\omega^2}} = \frac{\omega^2 - \omega_q^2}{\omega^2}$$

$$= \frac{(\omega - \omega_q)(\omega + \omega_q)}{\omega^2}$$

$$\omega_q^2 = \omega_p^2 + \frac{3}{5} (v_F q)^2 \qquad \boxed{\approx \frac{2}{\omega_q} (\omega - \omega_q)}$$

Règle de somme f :

$$\int_0^\infty \frac{d\omega'}{2\pi}\,\frac{\omega'}{2}\,\chi_{nn}(\omega') = \frac{nq^2}{4m}$$

$$\frac{1}{\epsilon_L} = 1 - \frac{4\pi e^2}{q^2}\,\chi_{nn}$$

$$\mathrm{Im}\,\frac{1}{\epsilon_L} = -\frac{4\pi e^2}{q^2}\,\mathrm{Im}\,\chi_{nn}$$

$$\boxed{\int_0^\infty \frac{d\omega}{2\pi}\,\mathrm{Im}\left(\frac{1}{\epsilon_L(q,\omega)}\right)\omega = -\frac{4\pi e^2}{\cancel{q^2}}\,\frac{n\cancel{q^2}}{4m} = -\frac{\omega_p^2}{4}}$$

$$\int_0^\infty \frac{d\omega}{2\pi}\,\omega\,\mathrm{Im}\left(\frac{1}{\frac{2}{\omega_q}(\omega-\omega_q)+i\eta}\right)$$

$$= -\pi\int_0^\infty \frac{d\omega}{2\pi}\,\omega\,\delta\left(\frac{2}{\omega_q}(\omega-\omega_q)\right)$$

$$= -\cancel{\pi}\int_0^\infty \frac{d\omega}{2\cancel{\pi}}\,\omega\,\frac{\omega_q}{2}\,\delta(\omega-\omega_q) = -\frac{\omega_q^2}{4}$$

$$\omega_q^2 = \omega_p^2 + \frac{3}{5}(v_F q)^2$$

5.4 Propriétés à 1 particule (H·F)

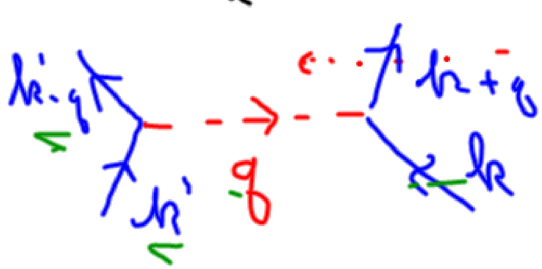
Approche variationnelle:

$$H_0 = \sum_{k\sigma} \epsilon_k \, c^{+}_{k\sigma} c_{k\sigma}$$

$$\boxed{H - H_0 = \frac{1}{2V} \sum_{k\sigma} \sum_{k'\sigma'} \sum_{q} c^{+}_{k\sigma} c^{+}_{k'\sigma'} V_q \, c_{k'+q\,\sigma'} c_{k+q\,\sigma}}$$

$$\frac{1}{2}\sum_{\sigma\sigma'} \int d^3r_1 \, d^3r_{1'} \, \psi^{+}_{\sigma}(r_1) \psi^{+}_{\sigma'}(r_{1'}) V(r_1 - r_{1'}) \psi_{\sigma'}(r_{1'}) \psi_{\sigma}(r_1)$$

$$\psi^{+}_{\sigma}(r_1) = \frac{1}{\sqrt{V}} \sum_{k} c^{+}_{k\sigma} e^{-ik\cdot r}$$



Variation:

Hamiltonien d'essai à 1 corps

Cherche $\boxed{\tilde{H}_0 = \sum_{k\sigma} \tilde{\epsilon}_k \, c^\dagger_{k\sigma} c_{k\sigma}}$

minimise:

$$\boxed{-T \ln Z_0 + \langle H - \tilde{H}_0 \rangle_0}$$

$$\boxed{-T\ln Z_0 = -T\sum_{k\sigma}\ln\left(1+e^{-\beta(\tilde{\epsilon}_k-\mu)}\right)}$$

$$\langle H-\tilde{H}_0\rangle_0 = \sum_{k\sigma}(\epsilon_k-\tilde{\epsilon}_k)\underbrace{\langle c^+_{k\sigma}c_{k\sigma}\rangle_0}_{f}$$

$$+\frac{1}{2V}\sum_{k\sigma k'\sigma'}\sum_q V_q\Big\{\langle c^+_{k\sigma}c_{k+q\sigma}\rangle_0\langle c^+_{k'\sigma'}c_{k'-q\sigma'}\rangle_0 \quad (q=0)$$

$$-\langle c^+_{k\sigma}c_{k'-q\sigma'}\rangle_0\langle c^+_{k'\sigma'}c_{k+q\sigma}\rangle_0\Big\}$$

$k = k'-q$

$k' = k+q$

$$\boxed{= \sum_{k\sigma}(\epsilon_k-\tilde{\epsilon}_k)f(\tilde{\xi}_k) - \cancel{2}\frac{1}{\cancel{2}V}\sum_{k'}\sum_q V_q\, f(\tilde{\xi}_{k'})f(\tilde{\xi}_{k'+q})}$$

$$\frac{\partial}{\partial \tilde{\epsilon}_k}(-T \ln Z_0) = \cancel{T}\, \frac{2\, e^{-\beta(\tilde{\epsilon}_k - \mu)}}{1 + e^{-\beta(\tilde{\epsilon}_k - \mu)}} \left(\cancel{\beta}\right)$$

$$= 2 f(\cancel{\tilde{\xi}_k})$$

$$+ \frac{\partial}{\partial \tilde{\epsilon}_k} \langle H - \tilde{H}_0 \rangle_0 = -2 f(\cancel{\tilde{\xi}_k})$$

$$+ \frac{\partial f(\tilde{\xi}_k)}{\partial \tilde{\epsilon}_k} \left[2 (\epsilon_k - \tilde{\epsilon}_k) - \frac{1}{V} \sum_q V_q \left(f(\tilde{\xi}_{k+q}) + f(\tilde{\xi}_{k-q}) \right) \right]$$

$$\tilde{\epsilon}_k = \epsilon_k - \frac{1}{V} \sum_q V_q\, f(\tilde{\xi}_{k+q})$$

$$\boxed{\tilde{\epsilon}_k = \epsilon_k - \int \frac{d^3k'}{(2\pi)^3} \frac{4\pi e^2}{|k - k'|^2} \frac{1}{e^{\beta(\tilde{\epsilon}_{k'} - \mu)} + 1}}$$

Autre dérivation :

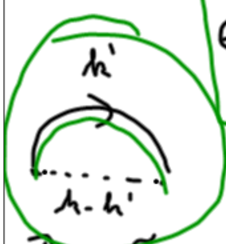
- Milieu effectif
- Théorie des perturbations renormalisée.
- H.F.

$$H = \tilde{H}_0 + \left(H_0 + V - \tilde{H}_0 \right)$$

$$\tilde{\Sigma} =$$

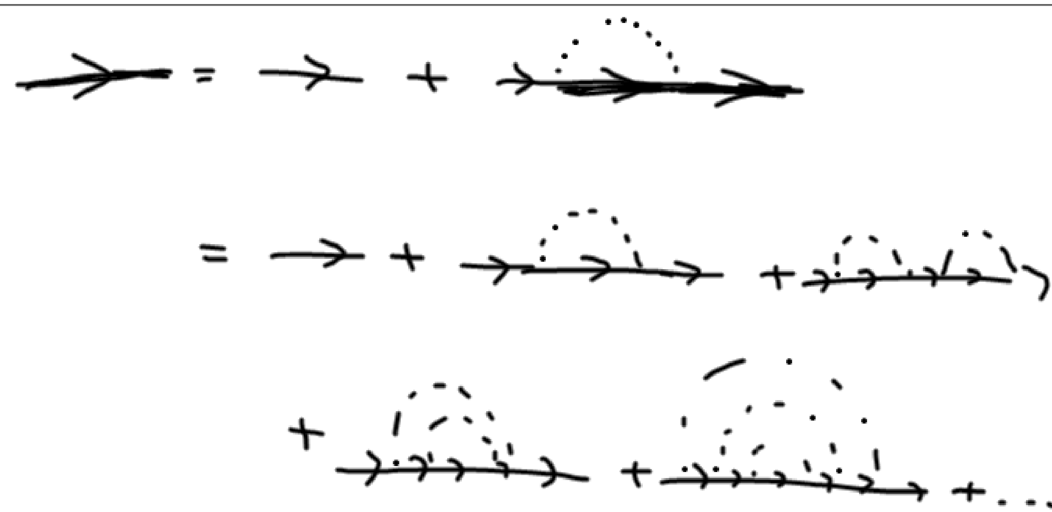
On pose : $\tilde{\Sigma} = 0$

$$\boxed{\epsilon_k - \tilde{\epsilon}_k + \Sigma^{(1)}(k) = 0}$$



$$\tilde{\epsilon}_k = \epsilon_k - \int \frac{d^3k'}{(2\pi)^3}\, T \sum_{ik_n'} e^{ik_n' \eta_+} \frac{V_{k-k'}}{ik_n' - (\tilde{\epsilon}_{k'} - \mu)}$$

$$\boxed{\tilde{\epsilon}_k = \epsilon_k - \int \frac{d^3k}{(2\pi)^3} \frac{4\pi e^2}{|k-k'|^2} \frac{1}{e^{\beta(\tilde{\epsilon}_{k'} - \mu)} + 1}}$$



diagrammes en arc-en-ciel

Pathologie :

Densité : (μ)

$$n = \frac{1}{V}\sum_\sigma \sum_k \langle c^+_{k\sigma} c_{k\sigma} \rangle$$

$$= \frac{1}{V}\lim_{\tau\to 0^-} \sum_\sigma \sum_k \mathcal{G}_\sigma(k,\tau)$$

$$= \frac{1}{V}\sum_\sigma \sum_k T \sum_{ik_n} \frac{e^{-ik_n\tau}}{ik_n - (\tilde{\epsilon}_k - \mu)}$$

$$\rightsquigarrow \quad n = 2\int \frac{d^3k}{(2\pi)^3} f(\tilde{\epsilon}_k - \mu)$$

$T = 0$

$$f : 0 \quad \text{pour} \quad \tilde{\epsilon}_k - \mu = 0$$

$$\rightsquigarrow \epsilon_{k_F} + \Sigma^{(1)}(k_F) - \mu = 0$$

$$n = 2\int \frac{d^3k}{(2\pi)^3} \theta(-|k| + k_F)$$

Luttinger

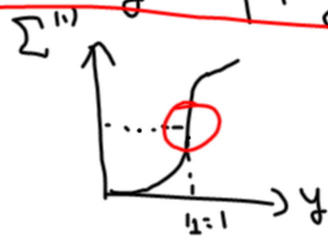
$$\Sigma^{(1)}(k) = -\int \frac{d^3k'}{(2\pi)^3}\,\frac{4\pi e^2}{|\underbrace{k-k'}|^2}\,\theta(k_F - |k|)$$

$$= -\frac{\cancel{4}\cancel{\pi}e^2}{\cancel{8}\pi^3}\cancel{2\pi}\int_0^{k_F} k'^2\,dk' \int_{-1}^{1}\frac{d(\cos\theta)}{k^2+k'^2-2kk'\cos\theta}$$

$$= -\frac{e^2}{\pi}\int_0^{k_F} k'\,dk'\,\frac{1}{-2k}\ln\left|\frac{(k'-k)^2}{(k'+k)^2}\right|$$

$$\boxed{\Sigma^{(1)}(k) = -\frac{e^2}{\pi}k_F\left[1+\frac{1-y^2}{2y}\ln\left|\frac{1+y}{1-y}\right|\right]}$$

$$\rightarrow \boxed{y \equiv \frac{k}{k_F}}$$



$$\frac{\Sigma^{(1)}(k_F)}{E_F} = \frac{-\frac{e^2}{\pi}k_F}{E_F} \propto \frac{me^2k_F}{k_F^2} \propto \frac{me^2}{k_F}$$

$$\propto \frac{1}{(k_F a_0)} \propto r_s \;!$$

$$\frac{m}{m^*} = \lim_{k\to k_F} \left.\frac{1+\frac{\partial}{\partial \xi_k}\mathrm{Re}\,\Sigma^R(k, E_k-\mu)}{1-\cancel{\frac{\partial}{\partial\omega}\mathrm{Re}\,\Sigma(k,\omega)}}\right|_{\omega = E_k-\mu}$$

0

$$\boxed{\frac{m}{m^*} = 1 + \frac{\partial k}{\partial \xi_k} \frac{\partial}{\partial k} \Sigma^{(1)}(k)}$$

$m^* = 0$

$\frac{\partial}{\partial k}\Sigma = \infty$

$$\frac{\partial}{\partial k}\Sigma^{(1)}(k) = \frac{\partial y}{\partial k} \frac{\partial}{\partial y} \Sigma^{(1)}(k)$$

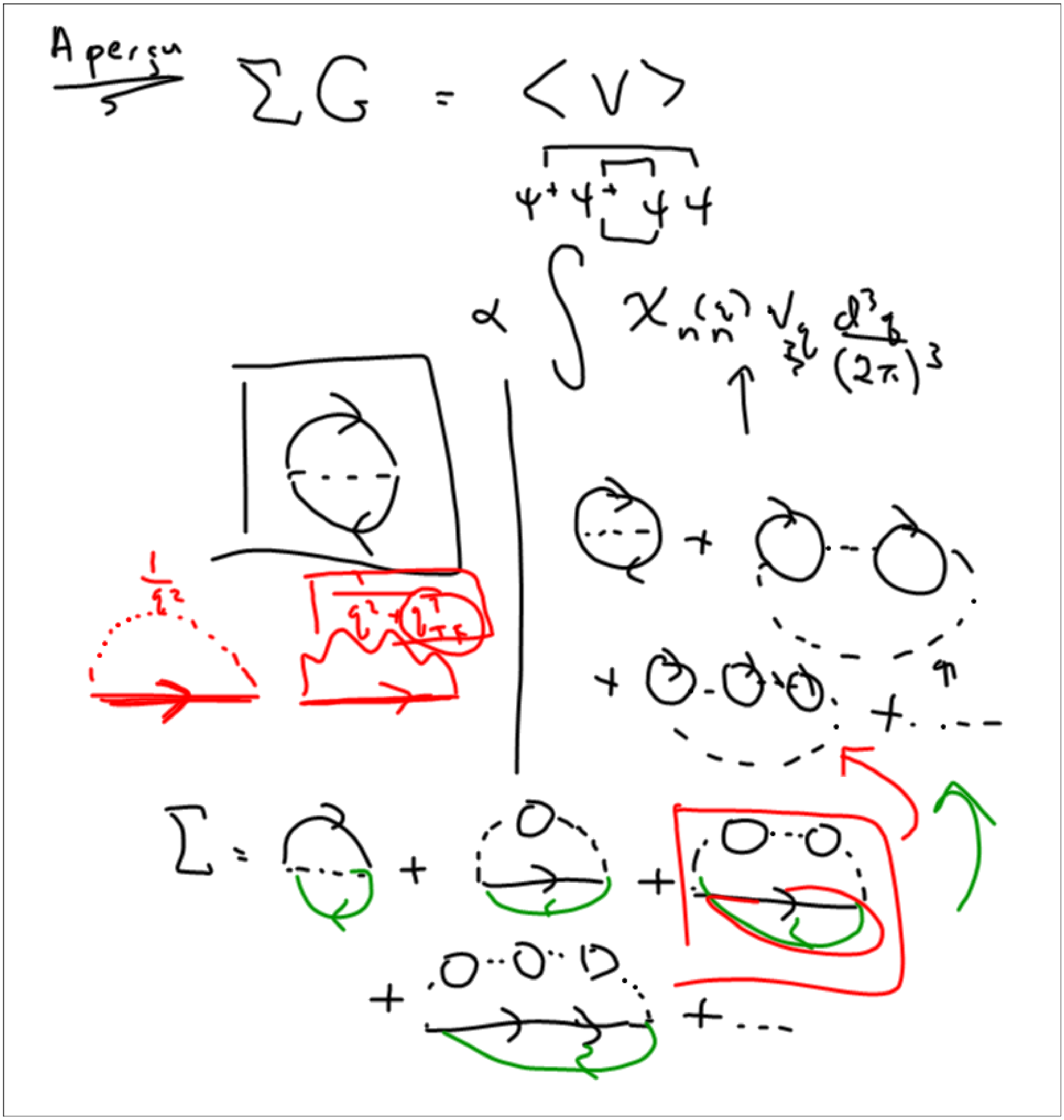
$$\frac{\partial}{\partial y}\Sigma^{(1)} = \frac{d}{dy} \frac{(1-y^2)}{2y} \ln\left|\frac{1+y}{1-y}\right|$$

$$\frac{d}{dy}\left(\frac{1-y^2}{2y}\ln(1-y)\right)$$

$$= \frac{d}{dy}\left[\left(\frac{1}{2y} - \frac{y}{2}\right)\ln(1-y)\right]$$

$$= \left(-\frac{1}{2y^2} - \frac{1}{2}\right) \ln(1-y)$$

$$(-)\left(\frac{1-y^2}{2y}\right)\frac{1}{1-y}$$


Aperçu
$\Sigma G = \langle V \rangle$
$\psi^\dagger \psi^\dagger \psi \psi$
$\propto \int \chi_{nn}(q)\, V_q \frac{d^3q}{(2\pi)^3}$
$\frac{1}{q^2}$
$\Sigma =$