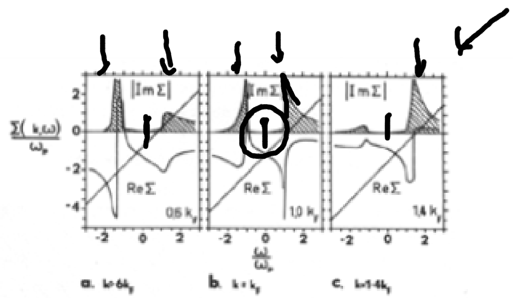

Figure 41-1 Real and imaginary part of the RPA self-energy for three wave vectors, in units of the plasma frequency. The chemical potential is included in ReΣ. The straight line that appears on the plots is $\omega - \varepsilon_{\mathbf{k}}$. Taken from B.I. Lundqvist, Phys. Kondens. Mater. **7**, 117 (1968). $r_s = 5$?

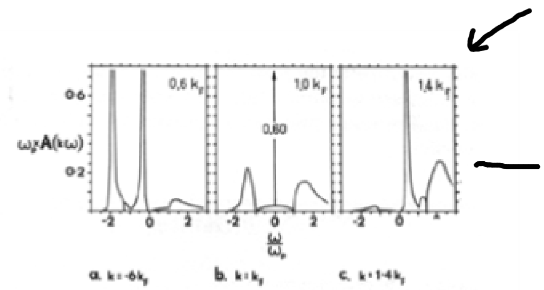

Figure 41-2 RPA spectral weight, in units of the inverse plasma frequency. Taken from B.I. Lundqvist, Phys. Kondens. Mater. **7**, 117 (1968).

41. Physique : propriétés à 1 particule

1. Poids spectral
→ 2. Interp. physique
→ 3. Liquide de Fermi
→ 4. Énergie libre
5. Comparaison avec expérience

VI. Fermions sur réseau: Hubbard et Mott

44. Densité fonctionnelle

1. Fondamental est une fonctionnelle de $n(\vec{r})$
2. Kohn. Sham
3. T finie

45. Modèle de Hubbard

1. $U=0$ 2. $t=0$

46. TPSC - ACDP

47. DMFT - TCMD

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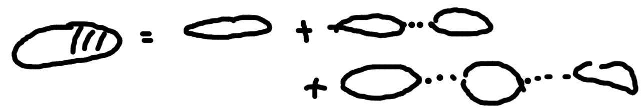
41.2 Interp. physique



$$\Sigma(k, ik_n) = \Sigma_{HF} + \int \frac{d^3q}{(2\pi)^3}\, T\sum_{iq_n} V_q\, \chi_{nn}(q, iq_n)\, V_q\, \frac{1}{ik_n + iq_n - \zeta_{k+q}}$$

$$= \Sigma_{HF} + \int \frac{d^3q}{(2\pi)^3}\, T\sum_{iq_n} \int \frac{d\omega'}{\pi}\, \frac{V_q\, \chi''_{nn}(q,\omega')\, V_q}{\omega' - iq_n}\, \frac{1}{ik_n + iq_n - \zeta_{k+q}}$$

$$T\sum_{iq_n} \frac{1}{\omega' - iq_n}\, \frac{1}{ik_n + iq_n - \zeta_{k+q}} = T\sum_{iq_n} \left[\frac{1}{\omega' - iq_n} + \frac{1}{ik_n + iq_n - \zeta_{k+q}} \right] \frac{1}{\omega' + ik_n - \zeta_{k+q}}$$

$$= \frac{n_B(\omega') + f(\zeta_{k+q})}{ik_n + \omega' - \zeta_{k+q}}$$

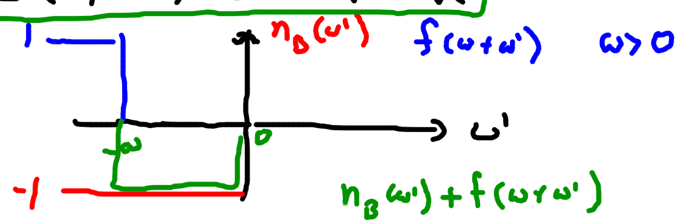
$$\Sigma_{HF} + \int \frac{d^3q}{(2\pi)^3} \int \frac{d\omega'}{\pi}\, \frac{\chi''_{nn}(q,\omega')\, V_q^2}{ik_n + \omega' - \zeta_{k+q}} \left[n_B(\omega') + f(\zeta_{k+q}) \right]$$

$ik_n \to \omega + i\eta$

$$\Sigma''(k,\omega) = -\pi \int \frac{d^3q}{(2\pi)^3} \int \frac{d\omega'}{\pi}\, V_q^2\, \chi''_{nn}(q,\omega') \left[n_B(\omega') + f(\omega+\omega') \right] \delta(\omega + \omega' - \zeta_{k+q})$$

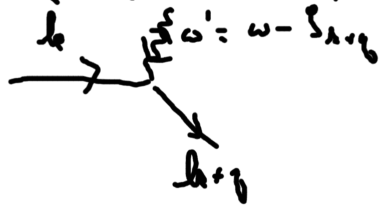
à $T = 0$ et $\omega = 0$ $\boxed{\Sigma''(k, \omega=0) = 0 \quad \forall\, k}$

$$n_B(\omega') = \frac{1}{e^{\beta\omega'} - 1}$$



$\omega > 0$ $\quad \omega' \to -\omega'$

$$(1 + n_B(\omega'))(1 - f(\zeta_{k+q})) + n_B(\omega')\, f(\zeta_{k+q})$$



$$\delta(\omega+\omega'-\xi_{k+q}) = \delta\left(\omega+\omega'-\cancel{\frac{k_F^2}{2m}}-\frac{k_F q}{m}-\frac{q^2}{2m}+\cancel{\mu}\right) \qquad \boxed{k=k_F}$$

$$\delta(ax) = \frac{1}{|a|}\delta(x)$$

$$\boxed{\frac{q_\parallel^2+q_\perp^2}{2m}} \qquad \boxed{q_\parallel \, , \, q_\perp} \qquad \boxed{\frac{k_F q_\parallel}{m}}$$

$$\Sigma''(k_F,\omega) = -\frac{\pi}{2\pi}\frac{m}{k_F}\int\frac{d^2q_\perp}{(2\pi)^2}\int\frac{d\omega'}{\pi}V_q^2\left[\frac{\chi''_{nn}(q,\omega')}{\omega'}\right]\left[n_B(\omega')+f(\omega+\omega')\right]\omega'$$

$$\int\frac{d^2q_\perp}{(2\pi)^2}\left[\frac{\chi''_{nn}(q_\perp,q_\parallel,\omega')}{\omega'}\right] = A(k_F)$$

$$\int\frac{d\omega'}{\pi}\,\omega'\left[n_B(\omega')+f(\omega+\omega')\right] \xrightarrow[T=0]{} \int_{-\omega}^{0}\frac{d\omega'}{\pi}\,\omega' = -\frac{\omega^2}{2\pi}$$

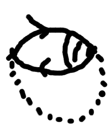
$$= -\frac{1}{2\pi}\left[\omega^2+(\pi T)^2\right]$$

41.4 Energie libre

$$Z = \mathrm{Tr}\left[e^{-\beta(\hat{T} + \lambda \hat{V} - \mu N)}\right]$$

$$\frac{\partial F}{\partial \lambda} = \langle V \rangle_\lambda \Rightarrow F = F_0 + \int_0^1 d\lambda \, \frac{1}{\lambda} \langle \lambda V \rangle_\lambda$$

$$\langle \lambda V \rangle = \int d1\, d2 \, \langle T_\tau \psi^+(1^+) \psi^+(2^+) \lambda V(1-2) \psi(2) \psi(1) \rangle_\lambda$$

 $\rightarrow \sum_q V_q \, \chi^\lambda_{nn}(q)$

$$\boxed{\chi^\lambda_{nn}(q) = \frac{\chi^0_{nn}}{1 + \lambda V_q \chi^0_{nn}}}$$

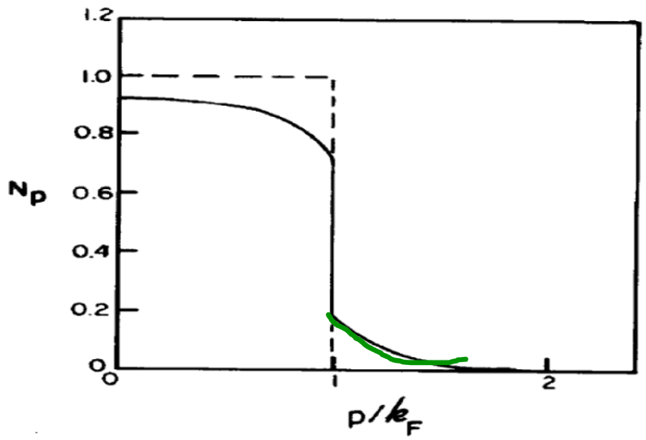
$$E_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - 0.17 r_s \left(\ln r_s + 0.2\right) \frac{k_F k}{2m} + cst$$

appearing in this expression is now obvious

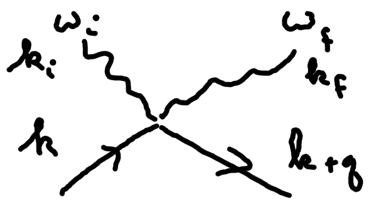
$$m^* = \frac{m}{1 - 0.08 r_s \left(\ln r_s + 0.2\right)}$$

cattering rate for $\omega = E_{\mathbf{k}} - \mu$ we find

$$\Gamma_{\mathbf{k}} \left(E_{\mathbf{k}} - \mu\right) = 0.25 r_s^{1/2} \frac{(k - k_F)^2}{2m}$$



r_s	Z_{RPA}
0	1
1	0.859
2	0.768
3	0.700
4	0.646
5	0.602
6	0.568



$\omega_f - \omega_i = \omega$

$k_f - k_i = q$

Effet Compton

$$\frac{d^2\sigma}{d\omega\, d\Omega} \propto \int \frac{d^3k}{(2\pi)^3}\, n_k\, \delta(\omega + \epsilon_k - \epsilon_{k+q})$$

$$\propto \int k^2 dk \int_{-1}^{1} d(\cos\theta)\, n_k\, \delta\left(\omega - \frac{q^2}{2m} - \frac{kq}{m}\cos\theta\right)$$

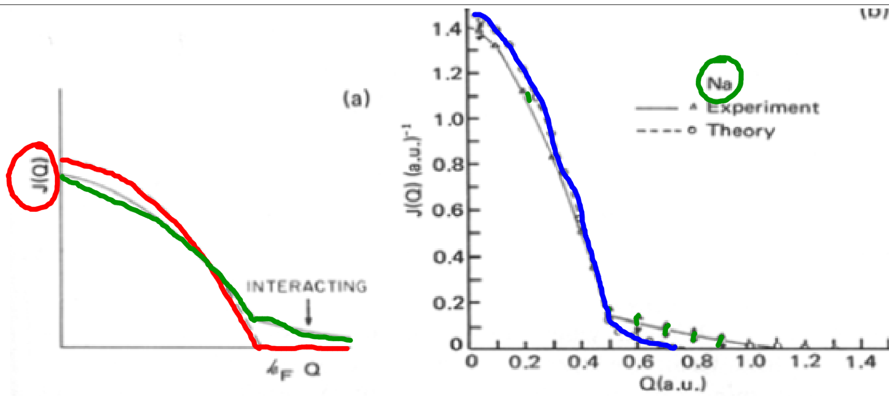
$$\int k^{\cancel{2}} dk \int_{-1}^{1} d(\cos\theta)\, n_k\, \frac{m}{\cancel{k}q}\, \delta\left(\left(\frac{\omega - \frac{q^2}{2m}}{\frac{kq}{m}}\right) - \cos\theta\right)$$

$$\frac{|Q|}{k} < 1 \qquad |Q| = \left|\left(\omega^2 - q^2/2m\right)\frac{m}{q}\right|$$

$$\int k\, dk\, n_k \left(\frac{m}{q}\right) \Theta\left(k - |Q|\right)$$

Cas sans interaction :

$$\int_{|Q|}^{k_F} k\, dk\, n_k\, \frac{m}{q} = \frac{k_F^2 - |Q|^2}{2q}\, m\, \Theta\left(k_F - |Q|\right)$$


(a)
J(Q)
INTERACTING
k_F Q
(b)
Na
Experiment
Theory
J(Q) (a.u.)$^{-1}$
Q(a.u.)
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
0.2
0.4
0.6
0.8
1.0
1.2
1.4

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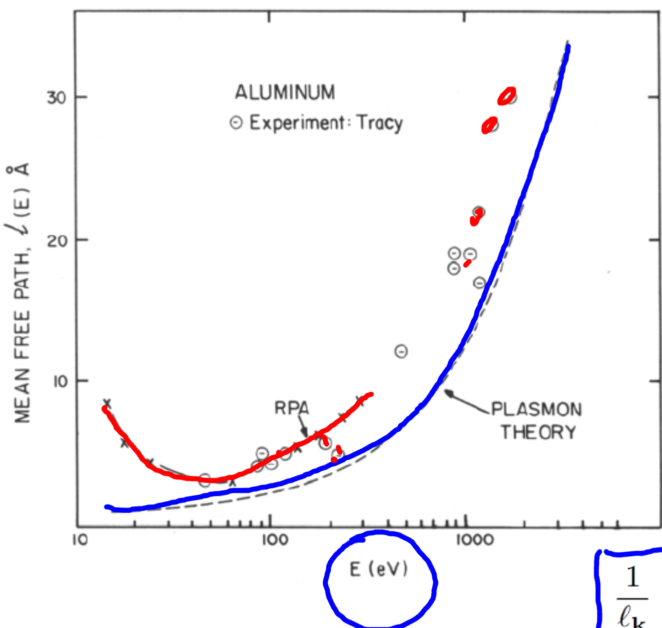

$$\frac{1}{\ell_{\mathbf{k}}} = \frac{\Gamma_{\mathbf{k}}}{v_{\mathbf{k}}} = \frac{1}{\tau_{\mathbf{k}} v_{\mathbf{k}}} = -\frac{2}{v_{\mathbf{k}}} \operatorname{Im} \Sigma\left(\mathbf{k}, \zeta_{\mathbf{k}}\right)$$

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44. Densité fonctionnelle

1. DFT

$$E = \min_{\Psi} \left[\frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right]$$

$$|\Psi\rangle = \sum_i a_i |i\rangle$$

$$\langle \Psi | H | \Psi \rangle = \sum_{ij} a_j^* a_i E_i \langle j | i \rangle$$

$$= \sum_i |a_i|^2 E_i$$

$$\geq \left(\sum_i |a_i|^2 \right) E_0$$

$$H = \hat{T}_e + \hat{V} + \hat{V}_\ell$$

$$\langle \Psi | \hat{V}_\ell | \Psi \rangle = \langle \Psi | \int d^3r \int d^3r' \sum_\sigma \psi_\sigma^+(r) \psi_\sigma(r) \frac{e^2}{4\pi\epsilon_0 |r - r'|} n_\ell(r') | \Psi \rangle$$

$$= \int d^3r \, n(\vec{r}) V_\ell(\vec{r})$$

$$n(\vec{r}) = \langle \Psi | \sum_\sigma \psi_\sigma^+(r) \psi_\sigma(r) | \Psi \rangle$$

$$E = \min_{n(r)} \boxed{\min_{\Psi \to n(\vec{r})}} \left[\boxed{\langle \Psi | \hat{T}_c + \hat{V} | \Psi \rangle} + \int d^3r \; n(r) V_\ell(r) \right]$$

$$E = \min_{n(\vec{r})} \left[F[n] + \int d^3r \; n(r) V_\ell(r) \right]$$

$$\boxed{F[n] = \min_{\Psi \to n(r)} \langle \Psi | \hat{T}_c + \hat{V} | \Psi \rangle}$$

$\langle \Psi | \hat{T} | \Psi \rangle$

$$\frac{k_F^2(r)}{2m}$$

exemple

$F[n]$

$$= \int d^3r \; A(r) \, n(\vec{r})$$

$$2 \int_0^{k_F(r)} \frac{d^3k}{(2\pi)^3} \frac{k^2}{2m} + \int d^3r \, d^3r' \, B(r-r') n(r) n(r') + \int d^3r \, C(r) \left(\nabla n(r)\right)^2$$

44.2 Kohn-Sham

$$\boxed{n(r) = \sum_{i=1}^{N/2} \sum_{\sigma} |\phi^{KS}_{i,\sigma}(r)|^2}$$

$$\boxed{\langle \Psi | \sum_\sigma \psi^\dagger_\sigma(r) \psi_\sigma(r) | \Psi \rangle}$$

$$|\Psi\rangle = a^\dagger_1 a^\dagger_2 \dots |0\rangle$$

Approximation pour $\langle \hat\Psi | \hat T_e | \hat\Psi \rangle$

$$= \sum_{i=1}^{N/2} \sum_\sigma \int d^3r \, \phi^{KS}_{i,\sigma} \left(\frac{-\nabla^2}{2m} \right) \phi^{KS}_{i,\sigma}$$

$\vec B = 0$

ϕ réels

. .

$$F[n] = \min_{\substack{KS \\ \to n}} \left[\langle \Psi | \hat T_e | \Psi \rangle_{KS} \right] + V_{Hartree}[n] + E_{xc}[n]$$

$$E_{xc} = \min_{\substack{K.S. \\ \to n}} \left(-\frac{1}{2} \int d^3r\, d^3r' \sum_{\sigma\sigma' ij} \phi^{KS}_{i\sigma}(r) \phi^{KS}_{j\sigma}(r) \frac{e^2}{4\pi\epsilon_0 |r-r'|} \phi^{KS}_{j\sigma'}(r') \phi^{KS}_{i\sigma'}(r') \right)$$

$$+ \int d^3r \, C^x n(r)^{4/3}$$