Ecole d'été 2014

04 mai 2014

①

A.1 Matrice densité:

$$\langle\psi|O|\psi\rangle = \sum_{ij} \langle\psi|i\rangle\langle i|O|j\rangle\langle j|\psi\rangle$$
$$= \sum_{ij} \langle j|\psi\rangle\langle\psi|i\rangle\langle i|O|j\rangle$$
$$= \sum_{ij} \langle j|\rho|i\rangle\langle i|O|j\rangle$$
$$= \mathrm{Tr}[\rho O]$$

$\rho \equiv |\psi\rangle\langle\psi|$ pure

$\rho^2 = 1$

Mixture

$$\rho = \sum_n p_n |\psi_n\rangle\langle\psi_n|$$

A.2 stat. mech

$$p_n = \frac{e^{-\beta(E_n - \mu N_n)}}{Z} = e^{-\beta(\hat{H} - \mu\hat{N})}$$

$$S = -k_B\,\mathrm{Tr}[\rho \ln \rho]$$

A.3 Legendre transforms:

$dE = TdS - pdV \qquad p = -\left(\frac{\partial E}{\partial V}\right)_S$

$d(E - TS) = -SdT - pdV \qquad p = -\left(\frac{\partial F}{\partial V}\right)_T$

$\longrightarrow T = \left(\frac{\partial E}{\partial S}\right)_V$

$$F(T,V) = \min_S \left(E(S) - TS\right)$$

$$\partial L = p\,d\dot{q} + \dot{p}\,dq$$
$$H = p\dot{q} - L$$
$$\dot{p} = \left(\frac{\partial L}{\partial q}\right)_{\dot{q}} = -\left(\frac{\partial H}{\partial q}\right)_p$$

24 mai 2014 ②

59. Second Quantization

59.1 States:

$$\langle \alpha_i | \alpha_j \rangle = \delta_{ij}$$

$$|\alpha_1 \alpha_2\rangle = -|\alpha_2 \alpha_1\rangle$$

ptcle 1 Ptcle 2

$$|\alpha_1 \alpha_2\rangle = \frac{1}{\sqrt{2}}\left(|\alpha_1\rangle \otimes |\alpha_2\rangle - |\alpha_2\rangle \otimes |\alpha_1\rangle\right)$$

$$a^+_{\alpha_1}|0\rangle = |\alpha_1\rangle$$

$$a^+_{\alpha_1} a^+_{\alpha_2}|0\rangle = |\alpha_1 \alpha_2\rangle$$

$$\boxed{\{a^+_{\alpha_1}, a^+_{\alpha_2}\} = 0 \quad | \quad \{a_{\alpha_1}, a_{\alpha_2}\} = 0}$$

$$a^+_{\alpha_1} a^+_{\alpha_2} = -a^+_{\alpha_2} a^+_{\alpha_1}$$

- Works if interchange 2 in the list
- Arbitrary initial order

Annihilation

$$\langle \alpha_1 | = \langle 0 | a_{\alpha_1}$$

$$\langle \alpha_1 | 0 \rangle = \langle 0 | a_{\alpha_1} | 0 \rangle = 0 \Rightarrow a_{\alpha_1}|0\rangle = 0$$

$$\langle \alpha_i | \alpha_j \rangle = \delta_{ij} \Rightarrow \langle 0 | a_{\alpha_i} a^+_{\alpha_j} | 0 \rangle = 0$$

$$\boxed{\{a_{\alpha_i}, a^+_{\alpha_j}\} = a_{\alpha_i} a^+_{\alpha_j} + a^+_{\alpha_j} a_{\alpha_i} = \delta_{ij}}$$

$$\hat{n}_{\alpha_i} = a^+_{\alpha_i} a_{\alpha_i}$$

$$\cancel{\hat{n}_{\alpha_i} a^+_{\alpha_j} = a^+_{\alpha_i} a_{\alpha_i} a^+_{\alpha_j}}$$

$$\cancel{= -a^+_{\alpha_i} a^+_{\alpha_j} a_{\alpha_i} + a^+_{\alpha_i} \delta_{ij}}$$

$\alpha_j \neq \alpha_i$

$$\hat{n}_{\alpha_i} a^+_{\alpha_i}|0\rangle = a^+_{\alpha_i} a_{\alpha_i} a^+_{\alpha_i}|0\rangle = -a^+_{\alpha_i} a^+_{\alpha_i} \overset{=0}{a_{\alpha_i}|}$$

$$\hat{n}_{\alpha_i} (a^+_{\alpha_j} a^+_{\alpha_k} \cdots a^+_{\alpha_i} \cdots a^+_{\alpha_\ell}) |0\rangle$$

$$= (a^+_{\alpha_j} a^+_{\alpha_k} \cdots \underbrace{\hat{n}_{\alpha_i} a^+_{\alpha_i}}_{\downarrow} \cdots a^+_{\alpha_\ell}) |0\rangle$$

$$a^+_{\alpha_i} a_{\alpha_i} a^+_{\alpha_i} = a^+_{\alpha_i} - \underbrace{a^+_{\alpha_i} a^+_{\alpha_i} a_{\alpha_i}}_{0}$$

$$= a^+_{\alpha_j} a^+_{\alpha_k} \cdots a^+_{\alpha_i} \cdots a^+_{\alpha_\ell} |0\rangle$$

59.2 Change of basis

$$|\mu_m\rangle = \sum_i |\alpha_i\rangle \langle \alpha_i | \mu_m \rangle$$

$$c^+_{\mu_m} = \sum_i a^+_{\alpha_i} \langle \alpha_i | \mu_m \rangle$$

59.2.1 Position basis

Momentum

$$\{ c_{\mu_m}, c^+_{\mu_n} \} = \langle \mu_m | \mu_n \rangle = \delta_{\mu_m \mu_n}$$

$$\{ c_k, c^+_{k} \} = \delta_{k,k'}$$

$$\psi^+(r) |0\rangle = |r\rangle$$

59.2.2 Wave function

$$\boxed{\langle 0 | \{ \psi(r), \psi^+(r') \} |0\rangle = \langle r | r' \rangle = \delta(r-r')}$$

$$\langle \alpha_1 \alpha_2 | = (a^+_{\alpha_1} a^+_{\alpha_2} |0\rangle)^+ = \langle 0 | a_{\alpha_2} a_{\alpha_1}$$

$$\langle r_1 r_2 \cdots r_{N-1} r_N | \alpha_1 \alpha_2 \cdots \alpha_N \rangle = \langle 0 | \psi(r_N) \cdots \psi(r_2) \psi(r_1) a^+_{\alpha_1} \cdots a^+_{\alpha_N} |0\rangle$$

$$\psi(r) = \sum_i \langle r | \alpha_i \rangle a_{\alpha_i}$$

$$= \sum_i \varphi_{\alpha_i}(r) a_{\alpha_i} \Rightarrow$$

$$= \sum_P \epsilon_P \, \phi_{\alpha_{P(1)}}(r_1)\, \phi_{\alpha_{P(2)}}(r_2) \cdots \phi_{\alpha_{P(N)}}(r_N)$$

$$= \det \begin{bmatrix} \phi_{\alpha_1}(r_1) & \phi_{\alpha_1}(r_2) & \cdots & \phi_{\alpha_1}(r_N) \\ \phi_{\alpha_2}(r_1) & \phi_{\alpha_2}(r_2) & \cdots & \phi_{\alpha_2}(r_N) \\ \vdots & & & \\ \phi_{\alpha_N}(r_1) & \phi_{\alpha_N}(r_2) & \cdots & \phi_{\alpha_N}(r_N) \end{bmatrix}$$

59.3

One-body operators

$$\hat{U}\,|\alpha_i\rangle = U_{\alpha_i}|\alpha_i\rangle = \langle \alpha_i|\hat{U}|\alpha_i\rangle\,|\alpha_i\rangle$$

$$\left(V(\vec{R}_1) + V(\vec{R}_2) + V(\vec{R}_3)\right)|r\, r'\, r''\rangle$$

Position in many-body

$$= \left(V(r) + V(r') + V(r'')\right)|r\, r'\, r''\rangle$$

$$\sum_m U_{\alpha_m}\hat{n}_{\alpha_m}|\alpha_i\, \alpha_j\, \alpha_k \cdots\rangle$$

$$\downarrow$$

$$\sum_m \langle \alpha_m|\hat{U}|\alpha_m\rangle\,\hat{n}_{\alpha_m} = \sum_{ij} c_i^\dagger \langle i|\hat{U}|j\rangle c_j$$

Potential energy:

$$\boxed{\hat{V} = \int d^3r\, V(r)\, \psi^\dagger(r)\,\psi(r)}$$

Kinetic energy

$$\boxed{\hat{T} = -\frac{\hbar^2}{2m}\int d^3r\, \psi^\dagger(r)\,\nabla^2\psi(r)}$$

Two-body operators

Diagonal basis: $\frac{1}{2}\sum_{ij} \langle \alpha_i| \otimes \langle \alpha_j|V|\alpha_i\rangle \otimes |\alpha_j\rangle\left(\hat{n}_{\alpha_i}\hat{n}_{\alpha_j} - \delta_{ij}\hat{n}_{\alpha_i}\right)$

$$= \frac{1}{2}\sum_{ij}(\alpha_i\,\alpha_j|V|\alpha_i\,\alpha_j)\, a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} a_{\alpha_j} a_{\alpha_i}$$

$$\boxed{\hat{V}_{\text{coulomb}} = \frac{1}{2}\int dx \int dy\, v(x-y)\,\psi^\dagger(x)\,\psi^\dagger(y)\,\psi(y)\,\psi(x)}$$

60. Hubbard

60.1 Hubbard model

$$H = \sum_{\sigma} \sum_{ij} c^{+}_{i\sigma} \langle i | \hat{\mathcal{H}}' | j \rangle c_{j} + \frac{1}{2} \sum_{\sigma\sigma'} \sum_{ijkl} \langle i | \langle j | V | k \rangle | l \rangle$$

$$\hat{T} + \hat{V} - \mu \hat{N}$$

$$c^{+}_{i\sigma} c^{+}_{j\sigma'} c_{l\sigma'} c_{k\sigma}$$

$$\rightarrow \boxed{\sum_{\sigma} \sum_{ij} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{\sigma\sigma'} \underbrace{\sum_{i} U c^{+}_{i\sigma} c^{+}_{i\sigma'} c_{i\sigma'} c_{i\sigma}}_{\sum_i U n_{i\uparrow} n_{i\downarrow}}}$$

Size of Hilbert space 4^N

$U = 0$

$$|\Psi\rangle_{U=0} = c^{+}_{k_0\uparrow} c^{+}_{k_0\downarrow} c^{+}_{k_1\uparrow} c^{+}_{k_1\downarrow} \cdots c^{+}_{k_{N/2}\uparrow} c^{+}_{k_{N/2}\downarrow} |0\rangle$$

$$|\Psi\rangle_{t=0} = c^{+}_{R_0\uparrow} c^{+}_{R_1\downarrow} c^{+}_{R_2\downarrow} \cdots c^{+}_{R_N\uparrow} |0\rangle$$

$|\Psi\rangle_{t=0}$ not eigenstate of t_{ij}

$|\Psi\rangle_{U=0}$ not eigenstate with U

$\Rightarrow$ Ψ linear combination !

complex coefficients (except H real)

$\Rightarrow$ Quantum fluctuations

$\Rightarrow$ Mott insulators

$\Rightarrow$ Ferro, Antiferro, ... high T_c

61. Perturbation theory and time-ordered products

$$e^{-\beta(H_0+H_1-\mu N)} = e^{-\beta(K_0+K_1)} = e^{-\beta K}$$

$$\boxed{\begin{aligned} e^{-\beta K} &= e^{-\beta K_0}\,\hat{U}(\beta) \\ \hat{U}(\beta) &\equiv T_\tau\left[e^{-\int_0^\beta d\tau\, K_1(\tau)}\right] \\ \hat{K}_1(\tau) &= e^{\cancel{\beta} K_0 \tau} K_1 e^{-K_0\tau} \end{aligned}}$$

$[K_1, K_0] = 0$ recover trivial

<u>Proof:</u> $\dfrac{\partial \hat{U}(\tau)}{\partial \tau} = -K_1(\tau)\,\hat{U}(\tau)$

$\cancel{\frac{\partial}{\partial\tau}\left[e^{-\tau K_0}\right] U(\beta)}$ $\dfrac{\partial}{\partial \tau}\left[e^{-\tau K_0}\hat{U}(\tau)\right]$

$= -(K_0+K_1)\left[e^{-\tau K_0}\hat{U}(\tau)\right]$

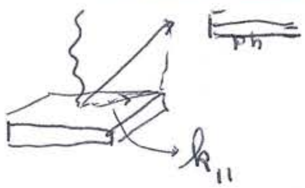
$$\hat{U}(\beta) - \hat{U}(0) = -\int_0^\beta K_1(\tau)\,\hat{U}(\tau)\,d\tau$$

$$\hat{U}(\beta) = 1 - \int_0^\beta K_1(\tau)\,d\tau + \int_0^\beta d\tau\, K_1(\tau)\int_0^\tau d\tau'\, K_1(\tau')$$
$$- \int_0^\beta d\tau\, K_1(\tau)\int_0^\tau d\tau'\, K_1(\tau')\int_0^{\tau'} d\tau''\, K_1(\tau'') + \cdots\cdots$$

62. Green functions contain useful information

Correlation functions for expt. (Spin!)

62.1 Photoemission + fermion correlation function



$$\frac{k^2}{2m} = E_{ph} + \omega + \mu - W$$

$$\sum_{m,n} \frac{e^{-\beta K_m}}{Z} \frac{2\pi}{\hbar} \left| \langle n| \otimes \langle k| \otimes \langle 0|_{em} \left(-\sum_{k'} \vec{j}_{k'} \cdot \vec{A}_{-k'} \right) |m\rangle \otimes |0\rangle \otimes |1_q\rangle_{em} \right|^2$$

$$\delta\left(\hbar\omega + \mu - (E_m - E_n)\right)$$

$$A_q \propto (a_q + a_q^\dagger) \qquad q \to 0$$

$$j_{k'=0} = e \sum_p \frac{\vec{p}}{m} c_p^\dagger c_p \qquad \text{spin dropped}$$

$$\boxed{\frac{\partial^2 \sigma}{\partial\Omega \partial\omega} \propto \sum_{mn} e^{-\beta K_m} \langle m | c^\dagger_{k_{\parallel}} | n \rangle \langle n | c_{k_{\parallel}} | m \rangle \, \delta\left(\omega - (K_m - K_n)\right)}$$

62.2 Definition

$$\mathcal{G}_{\alpha\beta}(\tau) = -\langle T_\tau c_\alpha(\tau) c^\dagger_\beta(0) \rangle$$

$$= -\langle c_\alpha(\tau) c^\dagger_\beta(0) \rangle \theta(\tau) + \langle c^\dagger_\beta(0) c_\alpha(\tau) \rangle \theta(-\tau)$$

Note: T_τ, perturbation theory

$$\langle O \rangle = \frac{\mathrm{Tr}\left[e^{-\beta \hat{K}} O\right]}{\mathrm{Tr}\left[e^{-\beta \hat{K}}\right]} \qquad \begin{aligned} c_\alpha(\tau) &= e^{\hat{K}\tau} c_\alpha e^{-\hat{K}\tau} \\ c^\dagger_\alpha(\tau) &= e^{\hat{K}\tau} c^\dagger_\alpha e^{-\hat{K}\tau} \end{aligned}$$

Note: $\hbar = 1$, $c^\dagger$ not adjoint

62.3 The Matsubara frequency representation is convenient

$$\mathcal{G}_{\alpha\beta}(\tau) = -\mathcal{G}_{\alpha\beta}(\tau-\beta)$$

Proof: $\tau > 0$

$$\mathcal{G}_{\alpha\beta}(\tau) = -\frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta\hat{K}}\, e^{\hat{K}\tau}\, c_\alpha\, e^{-\hat{K}\tau}\, c^+_\beta\right]$$

$$= -\frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta\hat{K}}\, c^+_\beta\, e^{(\tau-\beta)\hat{K}}\, c_\alpha\, e^{-\hat{K}\tau}\, e^{\beta\hat{K}}\right]$$

$$\boxed{\begin{aligned} \mathcal{G}_{\alpha\beta}(\tau) &= \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-ik_n\tau}\,\mathcal{G}_{\alpha\beta}(ik_n) \\ k_n &= (2n+1)\pi T \\ \mathcal{G}_{\alpha\beta}(ik_n) &= \int_0^\beta d\tau\, e^{ik_n\tau}\,\mathcal{G}_{\alpha\beta}(\tau) \end{aligned}}$$

62.4 $\mathcal{G}(ik_n)$ for $U=0$

$$\hat{K}_0 = \sum_p \xi_p\, c^+_p c_p \qquad \boxed{\mathcal{G}_k(\tau) = -\langle T_\tau\, c_k(\tau)\, c^+_k(0)\rangle}$$

$$\frac{\partial \mathcal{G}_k(\tau)}{\partial\tau} = -\delta(\tau)\,\langle\{c_k, c^+_k\}\rangle - \langle T_\tau\, \underbrace{\frac{\partial c_k(\tau)}{\partial\tau}}\, c^+_k(0)\rangle$$

$$= -\delta(\tau) - \xi_k\,\mathcal{G}_k(\tau)$$

$$\frac{\partial c_k(\tau)}{\partial\tau} = [K_0, c_k(\tau)] = -\xi_k\, c_k(\tau)$$

$$[AB, C] = A\{B,C\} - \{A,C\}B$$

$$(-ik_n + \xi_k)\,\mathcal{G}_k(ik_n) = -1$$

$$\boxed{\mathcal{G}_k(ik_n) = \frac{1}{ik_n - \xi_k}}$$

62.5 Spectral weight + relation to $\mathcal{G}_k(ik_n)$ and photoemission

$$\mathcal{G}_k(ik_n) = -\int_0^\beta d\tau\, e^{ik_n\tau} \sum_{n,m} \frac{e^{-\beta K_n}}{Z} \langle n| e^{K_n\tau} c_k e^{-K_m\tau} |m\rangle\langle m| c_k^\dagger |n\rangle$$

$$= \sum_{n,m} \frac{e^{-\beta K_n}}{Z} \frac{e^{\beta(K_n-K_m)}+1}{ik_n + K_n - K_m} \langle n| c_k |m\rangle\langle m| c_k^\dagger |n\rangle$$

Lehmann

$$\boxed{\mathcal{G}_k(ik_n) = \int \frac{d\omega}{2\pi} \frac{A_k(\omega)}{ik_n - \omega}}$$

$$A_k(\omega) = \sum_{m,n} \frac{e^{-\beta K_n}}{Z} \Big[\langle n| c_k^\dagger |m\rangle\langle m| c_k |n\rangle\, 2\pi\,\delta(\omega-(K_n-K_m)) + \langle n| c_k |m\rangle\langle m| c_k^\dagger |n\rangle\, 2\pi\,\delta(\omega-(K_m-K_n))\Big]$$

$$\frac{\partial^2\sigma}{\partial\Omega\,\partial\omega} \propto A_k(\omega)\, f(\omega)$$

$$\boxed{\int \frac{d\omega}{2\pi} A_k(\omega) = 1}$$ → Probability

62.6 A from $\mathcal{G}$: analytical continuation

$$A_k(\omega) = -2\,\mathrm{Im}\, G_k^R(\omega) = -2\,\mathrm{Im} \int \frac{d\omega'}{2\pi} \frac{A_k(\omega')}{\omega + i\eta - \omega'}$$

$$\lim_{\eta\to 0} \frac{1}{x+i\eta} = \frac{x-i\eta}{x^2+\eta^2} = \mathcal{P}\frac{1}{x} - i\pi\,\delta(x)$$

63 Self-energy and the effect of interactions

Non-interacting:

$A_k(\omega) = 2\pi\,\delta(\omega - \xi_k)$

63.1 The atomic limit $t=0$

$$\hat{K} = \sum_i \left(U n_{i\uparrow} n_{i\downarrow} - \mu n_{i\uparrow} - \mu n_{i\downarrow} \right)$$

$$\langle c_{k\uparrow}(\tau) c^{+}_{k\uparrow}(0)\rangle = \frac{1}{Z}\langle 0| e^{\hat{K}\tau} c_{\uparrow} e^{-\hat{K}\tau} |\uparrow\rangle\langle\uparrow| c^{+}_{\uparrow} |0\rangle$$

$$+ \frac{e^{\beta\mu}}{Z}\langle\downarrow| e^{\hat{K}\tau} c_{\uparrow} e^{-K\tau} |\downarrow\uparrow\rangle\langle\downarrow\uparrow| c^{+}_{k\uparrow} |\downarrow\rangle$$

$$= \frac{1}{Z} e^{\mu\tau} + \frac{e^{\beta\mu}}{Z} e^{-(U-\mu)\tau}$$

2 poles

$$\boxed{G^R_k(\omega) = \frac{1}{2}\left[\frac{1}{\omega + i\eta + \frac{U}{2}} + \frac{1}{\omega + i\eta - \frac{U}{2}}\right], \quad \mu = U/2}$$

63.2 Self-energy + atomic limit example

Def:
$$\boxed{G^R_{k\sigma}(\omega) \equiv \frac{1}{\omega + i\eta - \zeta_{k\sigma} - \Sigma^R_{k\sigma}(\omega)}}$$

$$\frac{1}{2\pi} A_{k\sigma}(\omega) = -\frac{1}{\pi}\operatorname{Im} G^R_{k\sigma}(\omega) = \frac{1}{\pi}\frac{-\operatorname{Im}\Sigma^R_{k\sigma}(\omega)}{(\omega - \zeta_{k\sigma} - \operatorname{Re}\Sigma^R_{k\sigma}(\omega))^2 + (\operatorname{Im}\Sigma^R_{k\sigma}(\omega))^2}$$

$$\left[G^{R^0}_{k\sigma}(\omega)\right]^{-1} = \omega + i\eta - \zeta_{k\sigma}$$

Dyson's equation:

$$\boxed{\left(\left[G^{R^0}_{k\sigma}(\omega)\right]^{-1} - \Sigma^R_{k\sigma}(\omega)\right) G^R_{k\sigma}(\omega) = 1}$$

63.3 A few properties:

$$\operatorname{Im}\Sigma^R(\omega) < 0 \quad \text{(poles in l.h.p.)}$$

$$\lim_{\omega\to\infty}\Sigma^R(\omega) = \text{Hartree-Fock}$$

63.4 Integrating out the bath: Anderson Impurity

$$H_I = H_f + H_c + H_{fc} - \mu N$$

$$K_f = \sum_\sigma (\epsilon - \mu) f^+_{i\sigma} f_{i\sigma} + U (f^+_{i\uparrow} f_{i\uparrow})(f^+_{i\downarrow} f_{i\downarrow})$$

$$K_c = \sum_\sigma \sum_k (\epsilon_k - \mu) c^+_{k\sigma} c_{k\sigma}$$

$$H_{fc} = \sum_\sigma \sum_k (V_{ki} c^+_{k\sigma} f_{i\sigma} + V^*_{ik} f^+_{i\sigma} c_{k\sigma})$$

$$\frac{\partial}{\partial\tau} \mathcal{G}_{ff}(\tau) = -\delta(\tau) - (\epsilon-\mu)\mathcal{G}_{ff}(\tau) \cancel{+ U \langle T_\tau f^+_{i\sigma} f_{i-\sigma}}$$

$$+ U \langle T_\tau f^+_{i-\sigma}(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) f^+_{i\sigma} \rangle - \sum_k V^*_{ik} \mathcal{G}_{cf}(k,i;\tau)$$

$$\frac{\partial}{\partial\tau} \mathcal{G}_{cf}(k,i;\tau) = -(\epsilon_k - \mu)\mathcal{G}_{cf}(k,i;\tau) - V_{ki}\mathcal{G}_{ff}(\tau)$$

$$\boxed{\Sigma_{ff}(ik_n)\mathcal{G}_{ff}(ik_n) = -U\int_0^\beta d\tau\, e^{ik_n\tau} \langle T_\tau f^+_{i-\sigma}(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) f^+_{i\sigma}\rangle}$$

$$\begin{bmatrix} ik_n - (\epsilon-\mu) - \Sigma_{ff}(ik_n) & -V^*_{ik} \\ -V_{ki} & ik_n - (\epsilon_k - \mu) \end{bmatrix} \begin{pmatrix} \mathcal{G}_{ff}(ik_n) \\ \mathcal{G}_{cf}(ik_n) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\boxed{\Big[ik_n - (\epsilon-\mu) - \underbrace{\sum_k V^*_{ik} \frac{1}{ik_n - (\epsilon_k - \mu)} V_{ki}}_{\Delta(ik_n)} \Big] \mathcal{G}_{ff}(ik_n) = 1 + \Sigma_{ff}(ik_n)\mathcal{G}_{ff}(ik_n)}$$

64. Many-particle correlation functions and Wick's theorem

$$\boxed{\begin{aligned}&\langle T_\tau\, \psi(\tau_1)\psi(\tau_2)\ldots\psi(\tau_n)\psi^+(\tau'_n)\ldots\psi^+(\tau'_2)\psi^+(\tau'_1)\rangle \\ &= (-1)^n \det \begin{bmatrix} \mathcal{G}(\tau_1,\tau'_1) & \mathcal{G}(\tau_1,\tau'_2) & \ldots & \mathcal{G}(\tau_1,\tau'_n) \\ \vdots & & & \\ \mathcal{G}(\tau_n,\tau'_1) & \ldots & \ldots & \mathcal{G}(\tau_n,\tau'_n)\end{bmatrix}\end{aligned}}$$

$$Z = \sum_{n_1=0}^{1}\sum_{n_2=0}^{1} \langle n_1 n_2| e^{-\beta \xi_1 c_1^+ c_1} \underset{\overset{\uparrow}{|n_1 n_2\rangle\langle n_1 n_2|}}{} e^{-\beta \xi_2 c_2^+ c_2} |n_1 n_2\rangle$$

$$= \sum_{n_1=0}^{1}\sum_{n_2=0}^{1}$$

$$= \sum_{n_1=0}^{1}\sum_{n_2=0}^{1} \langle n_1| e^{-\beta\xi_1 \hat{n}_1}|n_1\rangle \langle n_2| e^{-\beta \xi_2 \hat{n}_2}|n_2\rangle$$

$$= Z_1 Z_2$$

$$\langle O_1 O_2\rangle = \langle O_1\rangle\langle O_2\rangle$$

<u>Example:</u>

utiliser e

$$\langle a_\alpha^{+} a_\beta a_\gamma^+ a_\delta^+\rangle$$

$$= + \langle a_\beta a_\gamma^+\rangle\langle a_\alpha a_\delta^+\rangle - \langle a_\alpha a_\gamma^+\rangle\langle a_\beta a_\delta^+\rangle$$

25 mai 2014

65. Source fields to calculate many-body Green functions.

65.1 A simple example from classical stat. mech.

$$Z[h] = \mathrm{Tr}\left[e^{-\beta\left(K - \int dx\, h(x) M(x)\right)} \right]$$

with operators that commute

$$\frac{\delta}{\delta h(x_1)} \int dx\, h(x) M(x) = \int dx \frac{\delta h(x)}{\delta h(x_1)} M(x)$$

$$= M(x_1)$$

$$\frac{\delta h(x)}{\delta h(x_1)} = \delta(x_1 - x)$$

$$\frac{\delta^2 \ln Z}{\beta^2 \delta h(x_1) \delta h(x_2)} = \langle M(x_1) M(x_2) \rangle_h - \langle M(x_1)\rangle_h \langle M(x_2)\rangle_h$$

65.2 Green functions and higher order correlation functions

$$Z[\varphi] = \mathrm{Tr}\left[e^{-\beta K} \underbrace{T_\tau\, e^{-\psi^+(\bar{1})\varphi(\bar{1},\bar{2})\psi(\bar{2})}}_{S[\varphi]} \right]$$

$$\bar{1} \to \int d^3x_1 \int_0^\beta d\tau_1 \sum_{\sigma_1}$$

$$\boxed{\frac{\delta\varphi(\bar{1},\bar{2})}{\delta\varphi(1,2)} = \delta(\bar{1}-1)\,\delta(\bar{2}-2)}$$

$$\psi^+(1) = \psi^+_{\sigma_1}(x_1, \tau_1)$$

$$\boxed{\frac{-\delta \ln Z[\varphi]}{\delta\varphi(2,1)} = \mathcal{G}(1,2)_\varphi} = -\frac{\langle T_\tau S[\varphi]\, \psi(1)\psi^+(2)\rangle}{\langle T_\tau S[\varphi]\rangle}$$

$$= -\langle T_\tau \psi(1)\psi^+(2)\rangle_\varphi$$

$$\boxed{\frac{\delta \mathcal{G}(1,2)_\varphi}{\delta\varphi(3,4)} = \langle T_\tau \Psi(1)\Psi^+(2)\Psi^+(3)\Psi(4)\rangle_\varphi + \mathcal{G}(1,2)_\varphi\, \mathcal{G}(4,3)_\varphi}$$

66. Equations of motion for $\mathcal{G}_\varphi$ and Σ_φ

66.1 Hamiltonian and equs of motion for $\Psi(1)$

$$\frac{\partial \Psi(1)}{\partial \tau_1} = \frac{\nabla_1^2}{2m}\Psi(1) + \mu\Psi(1) - \Psi^+(\bar{2})\Psi(\bar{2})\,V(\bar{2}-1)\Psi(1)$$

$$V(1,2) = \frac{e^2}{4\pi\epsilon_0|x_1-x_2|}\,\delta(\tau_1-\tau_2)$$

66.2 Equations of motion for $\mathcal{G}_\varphi$ and def. of Σ_φ

$$-\left(\frac{\partial}{\partial\tau_1} - \frac{\nabla_1^2}{2m} - \mu\right)\mathcal{G}(1,2)_\varphi = \delta(1-2) + \phi(1,\bar{2})\mathcal{G}(\bar{2},2)_\varphi$$

$$- \langle T_\tau\left[\Psi^+(\bar{2}^+)\Psi(\bar{2})\,V(1-\bar{2})\,\Psi(1)\Psi^+(2)\right]\rangle_\varphi$$

$$\mathcal{G}_0^{-1}(1,\bar{2}) = -\left(\frac{\partial}{\partial\tau_1} - \frac{\nabla_1^2}{2m} - \mu\right)\delta(1-\bar{2})$$

$$\boxed{\left[\mathcal{G}_0^{-1}(1,\bar{2}) - \varphi(1,\bar{2}) - \Sigma(1,\bar{2})_\varphi\right]\mathcal{G}(\bar{2},2)_\varphi = \delta(1-2)}$$

$$\boxed{\begin{aligned} &= \Sigma(1,\bar{2})_\varphi\,\mathcal{G}(\bar{2},2)_\varphi \\ &= -\langle T_\tau\left[\Psi^+(\bar{2}^+)\Psi(\bar{2})\,V(1-\bar{2})\,\Psi(1)\Psi^+(2)\right]\rangle_\varphi \end{aligned}}$$

67. The General many-body problem

67.1 An integral equation for the 4-point function

$$\frac{\delta}{\delta\varphi}\left(\mathcal{G}^{-1}\mathcal{G}\right)=0$$

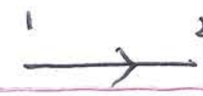
$$\frac{\delta\mathcal{G}^{-1}}{\delta\varphi}\mathcal{G}+\mathcal{G}^{-1}\frac{\delta\mathcal{G}}{\delta\varphi}=0$$

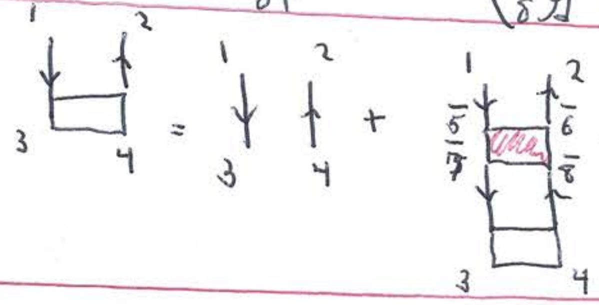
$$\frac{\delta\mathcal{G}}{\delta\varphi}=-\mathcal{G}\,\frac{\delta\mathcal{G}^{-1}}{\delta\varphi}\,\mathcal{G} \qquad \mathcal{G}^{-1}=\mathcal{G}_0^{-1}-\varphi-\Sigma$$

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

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

$\mathcal{G}(1,2)$





$$\frac{\delta\Sigma(\bar{5},\bar{6})}{\delta\mathcal{G}(\bar{7},\bar{8})}$$

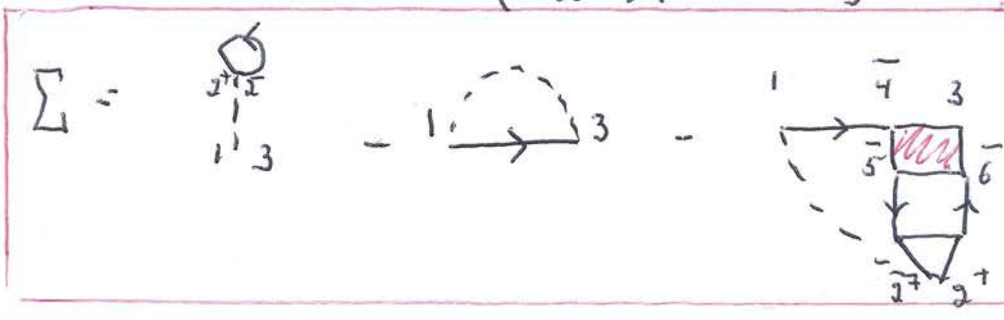
67.2 Self-energy from functional derivative

$$\Sigma=-V\left(\frac{\delta\mathcal{G}}{\delta\varphi}-\mathcal{G}\mathcal{G}\right)\mathcal{G}^{-1}$$

$$=-V\left(\mathcal{G}\,\frac{\delta\varphi}{\delta\varphi}\,\mathcal{G}+\mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\,\frac{\delta\mathcal{G}}{\delta\varphi}\right)\mathcal{G}\right)\mathcal{G}^{-1}$$

$-\mathcal{G}\mathcal{G}$

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



68. Long-range forces and GW

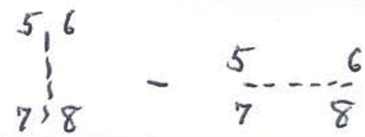
68.1 In space-time

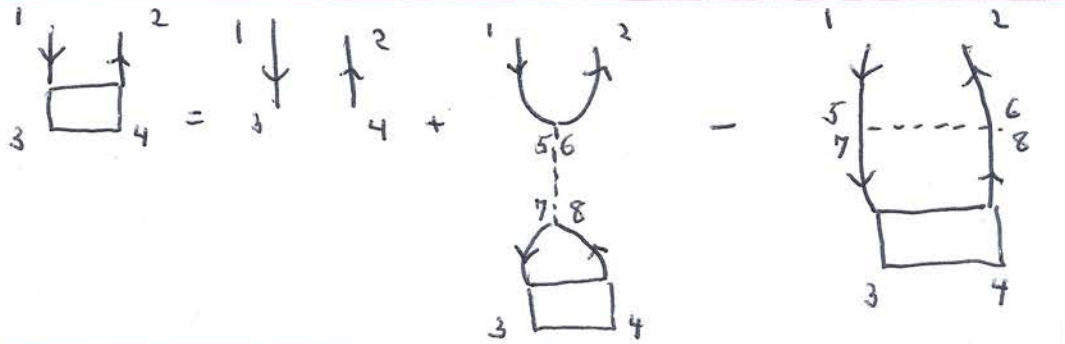
$\Sigma(1,3) =$

$\Sigma(5,6) =$

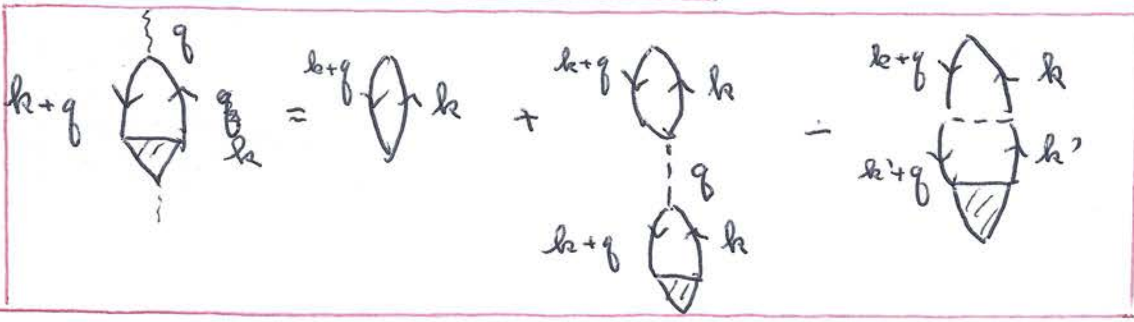
N.B. $\delta(5-6)$

$$\boxed{\frac{\delta \Sigma(5,6)}{\delta \mathcal{G}(7,8)} =}$$





68.2 In momentum-space with $\varphi = 0$



$$\chi_{nn}(1-2) = -\sum_{\sigma_1 \sigma_2} \frac{\delta \mathcal{G}(1,1^+)}{\delta \varphi(2^+,2)}$$

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

p. suivante

68.3 Density response in the RPA

$$-\sum_{\sigma_1\sigma_2} \frac{\delta \mathcal{G}(1,1^+)}{\delta \varphi(2^+,2)} = \sum_{\sigma_1\sigma_2} \langle T_\tau\, \psi^+(1^+)\psi(1)\, \psi^+(2^+)\psi(2)\rangle - n^2$$

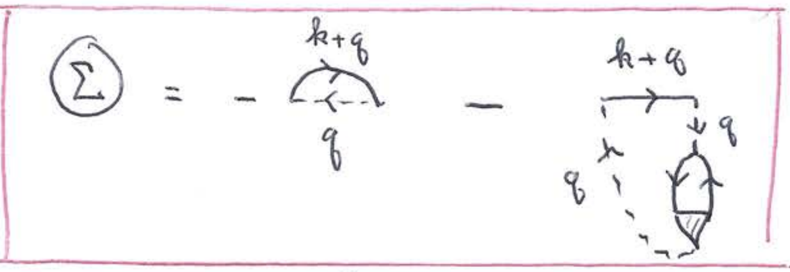
$$= \langle T_\tau\, n(1)\, n(2)\rangle - n^2$$

$$= \langle T_\tau\, (n(1)-n)\,(n(2)-n)\rangle$$

$$= \chi(1-2)$$

2 equs. p. précédente.

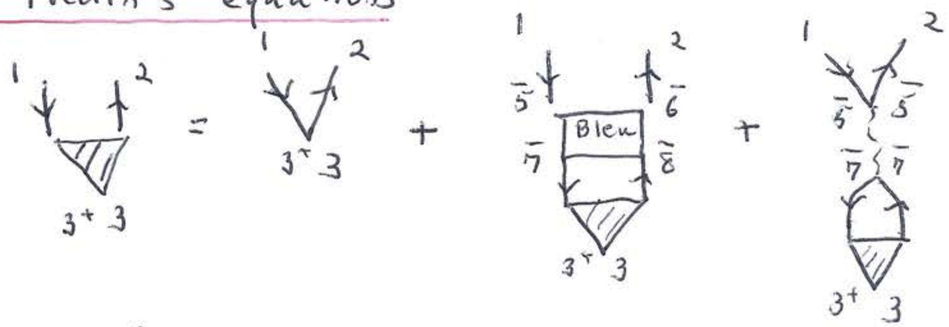
68.4 Σ and screening in the GW approximation

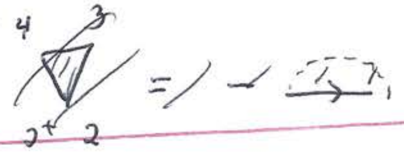


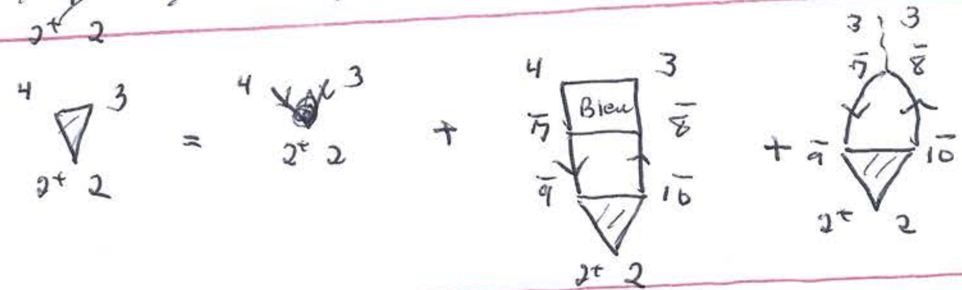
$$= -\int \frac{d^3 q}{(2\pi)^3}\, T \sum_{iq_n} \underbrace{V_q \left[1 - \frac{V_q\, \chi^0_{nn}(q, iq_n)}{1 + V_q\, \chi^0_{nn}(q, iq_n)}\right]} \mathcal{G}^0(k+q, ik_n + iq_n)$$

$$\frac{V_q}{1 + V_q\, \chi^0_{nn}(q, iq_n)} = \frac{V_q}{\frac{\epsilon(q, iq_n)}{\epsilon_0}}$$

68.5 Hedin's equations







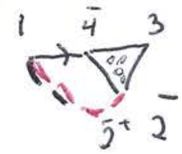
$$\Gamma(2^+,2;4,3) = I + \Gamma\mathcal{G}\mathcal{G}I + \Gamma\mathcal{G}\mathcal{G}V$$

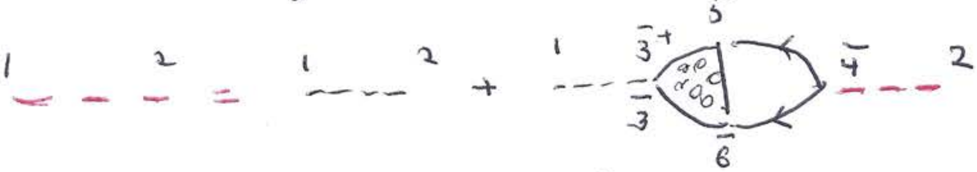
$$= (1-\mathcal{G}\mathcal{G}I-\mathcal{G}\mathcal{G}V)^{-1}$$

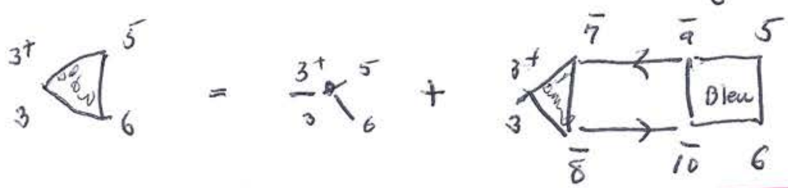
$$= (1-(1-\mathcal{G}\mathcal{G}I)^{-1}\mathcal{G}\mathcal{G}V)^{-1}(1-\mathcal{G}\mathcal{G}I)^{-1}$$

$$= (1-\Gamma\mathcal{G}\mathcal{G}V)^{-1}\Gamma$$

$\Sigma = -$  $= -\mathcal{G}V(1-\Gamma\mathcal{G}\mathcal{G}V)^{-1}\Gamma$

$\Sigma = -$ 





69. Luttinger Ward and related functionals.

$$F[\varphi] = -T \ln Z[\varphi]$$

$$\frac{1}{T}\frac{\delta F}{\delta \varphi(1,2)} = \mathcal{G}(2,1)$$

Legendre transform:

$$\boxed{\Omega[\mathcal{G}] = F[\varphi] - \mathrm{Tr}[\varphi \mathcal{G}]}$$ Kadanoff Baym Functional

$$\mathrm{Tr}[\varphi \mathcal{G}] = T\, \varphi(1,\bar{2})\, \mathcal{G}(\bar{2},\bar{1}) = T \sum_{ik_n} \sum_{k} [\quad]$$

$$\boxed{\frac{1}{T}\frac{\delta \Omega[\mathcal{G}]}{\delta \mathcal{G}(1,2)} = -\varphi(2,1) = \mathcal{G}^{-1}(2,1)_{\varphi} - \mathcal{G}_0^{-1}(2,1) + \Sigma(2,1)_{\varphi}}$$

$$\Omega[\mathcal{G}] = \mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_\infty}\right)\right] - \mathrm{Tr}\left[(\mathcal{G}_0^{-1} - \mathcal{G}^{-1})\mathcal{G}\right] + \Phi[\mathcal{G}]$$

$$\frac{1}{T}\frac{\delta \Phi[\mathcal{G}]}{\delta \mathcal{G}(1,2)} = \Sigma(2,1)$$

Explicit, universal functional of V:

$$\left.\frac{\partial \Omega_\lambda[\mathcal{G}]}{\partial \lambda}\right|_{\mathcal{G}} = \left.\frac{\partial F_\lambda[\varphi]}{\partial \lambda}\right|_{\phi} = \left.\frac{\partial \Phi_\lambda[\mathcal{G}]}{\partial \lambda}\right|_{\mathcal{G}}$$

$$= \frac{1}{\lambda}\langle \lambda \hat{V} \rangle_\lambda$$

70. A glance at coherent states functional integrals

70.1 Fermion coherent states

$c|\eta\rangle = \eta|\eta\rangle$ $\quad \{\eta_1, \eta_2\} = 0$ since $c_1 c_2 |\eta_1 \eta_2\rangle = -c_2 c_1 |\eta_1 \eta_2\rangle$

$\{\eta_i, \eta_i^+\} = 0$ since inside T_τ

$$|\eta\rangle = (1 - \eta c^+)|0\rangle$$

$$c|\eta\rangle = c|0\rangle + \eta c c^+ |0\rangle = \eta|0\rangle = \eta(1-\eta c^+)|0\rangle = \eta|\eta\rangle$$

anticommute.

70.2 Grassmann calculus

$$\int d\eta = 0 \qquad \int d\eta\, \eta = 1$$

$$\int \mathcal{D}\eta^+ \int \mathcal{D}\eta = \prod_i \int d\eta_i^+ \int d\eta$$

$$\boxed{\int \mathcal{D}\eta^+ \int \mathcal{D}\eta \; e^{-\eta^+ A \eta - \eta^+ J - J^+ \eta} = \det A \; e^{J^+ A^{-1} J}}$$

70.3 Recognizing H:

$$\int \mathcal{D}\eta^+ \int \mathcal{D}\eta \; e^{-S}$$

$$S = \int_0^\beta d\tau \left[\sum_\sigma \psi_\sigma^+(\tau) \frac{\partial}{\partial \tau} \psi_\sigma(\tau) + H\left(\psi_\sigma^+(\tau), \psi_\sigma(\tau)\right) \right]$$

$$p = \frac{\partial L}{\partial \dot{q}} \qquad \psi_\sigma^+(\tau) = \frac{\partial L}{\partial \dot{\psi}_\sigma(\tau)}$$