6 juin 2022

# Lectures : Why

## #1 Second quantization (45 min)

Useful if more than 1 Slater det.

## #2 Green's functions (45 min)

Necessary for P.T. ⇒ many methods
even DMFT non-perturbative.

## #3 Self-energy, Dyson's equation, atomic limit (90 min)

- GW
- Many-body P.T.

## #4 Coherent state functional integrals (90 min.)

- Derivation DMFT (Geo-ges)
- CTQMC (Ferrero)

## #5 Many-body perturbation theory (90 min)

- GW
- Luttinger-Ward

## #6 GW + TPSC (90 min)

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Cours #1, 45 min.

# Chap. 87 Second quantization

Summary

## 87.1 Creation-annihilation operators

$$\{a^{(+)}_{\alpha_1}, a^{(+)}_{\alpha_2}\} = 0 \qquad \{a_{\alpha_i}, a^+_{\alpha_j}\} = \delta_{ij}$$

Number operator

$$[n_\alpha, a^+_\alpha] = a^+_\alpha \qquad [n_\alpha, a_\alpha] = -a_\alpha$$

## 87.2 Change of basis

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

### 87.2.1 Position and momentum basis

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

$$c^+_k |0\rangle = |k\rangle$$

### 87.2.2 Wave-functions

$$\langle r_1, \ldots r_N | \alpha_1 \ldots \alpha_N \rangle =$$

$$\det \begin{bmatrix} \varphi_{\alpha_1}(r_1) & \varphi_{\alpha_1}(r_2) \ldots & \varphi_{\alpha_1}(r_N) \\ \vdots & & \\ \varphi_{\alpha_N}(r_1) & \varphi_{\alpha_N}(r_2) \ldots & \varphi_{\alpha_N}(r_N) \end{bmatrix}$$

## 87.3 One-body operators

$$\hat{V} = \sum_\sigma \int d^3r \, V(r) \, \psi^+_\sigma(r) \, \psi_\sigma(r) \qquad \hat{T} = \sum_\sigma \int d^3r \left(-\frac{\hbar^2}{2m}\right) \psi^+_\sigma(r) \nabla^2 \psi_\sigma(r)$$

## 87.4 Two-body operators

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

# 87 Second quantization

Why the name?

$$L \to p = \frac{\partial L}{\partial \dot q} \quad \frac{[q,p]}{i\hbar} \Rightarrow 1 \Leftarrow \{q,p\}_{p.b.}$$

$$\dot q = \frac{[q,H]}{i\hbar} \leftarrow \{q,H\}_{p.b}$$

$\downarrow$

apply that recipe to $\Psi$ and $E$

particles $\longrightarrow$ wave  wave $\longrightarrow$ particle.

Pedestrian approach: wave particle duality

## 87.1 Creation-annihilation operators

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

2 particules

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

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

Creation operator (Fock-space)

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

adds and antisymmetrices

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

(1) $$\boxed{0 = \{a^+_{\alpha_1}, a^+_{\alpha_2}\} \equiv a^+_{\alpha_1} a^+_{\alpha_2} + a^+_{\alpha_2} a^+_{\alpha_1}}$$

- Initial order arbitrary
- Works if interchange any two of list

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## Annihilation

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

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

## Final anticommutation

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

$$(2) \quad \boxed{\{a_{\alpha_i}, a^+_{\alpha_j}\} = \delta_{ij}}$$

## Number operator

$$\hat{n}_{\alpha_1} = a^+_{\alpha_1} a_{\alpha_1}$$

$$\hat{n}_{\alpha_1}|0\rangle = 0$$

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

$$= a^+_{\alpha_1}[1 - a^+_{\alpha_1} a_{\alpha_1}]|0\rangle = a^+_{\alpha_1}|0\rangle$$

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

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

if (2) applies. Works for any state.

$$\boxed{[\hat{n}_{\alpha_i}, a^+_{\alpha_j}]} = \delta_{ij}[a^+_{\alpha_i} a_{\alpha_i} a^+_{\alpha_i} - \underbrace{\cancel{a^+_{\alpha_i} a^+_{\alpha_i}}}_{0} a_{\alpha_i}]$$

$$= \delta_{ij}[a^+_{\alpha_i}(1 - a^+_{\alpha_i} a_{\alpha_i})] = \boxed{\delta_{ij} a^+_{\alpha_i}}$$

$$\boxed{[\hat{n}_{\alpha_i}, a_{\alpha_j}] = -a_{\alpha_j}}$$

## 87.2 Change of basis

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

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

$$\{a_{\mu_m}, a^+_{\mu_n}\} = \sum_{ij}\langle\mu_m|\alpha_i\rangle\{a_{\alpha_i}, a^+_{\alpha_j}\}\langle\alpha_j|\mu_n\rangle$$

$$= \langle\mu_m|\mu_n\rangle = \delta_{m,n}$$

### 87.2.1 Position-momentum basis

$$\{c_k, c^+_{k'}\} = \delta_{k,k'}$$ discrete on lattice.

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

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

### 87.2.2 Wave function

$$\langle r_1 r_2 \cdots r_N|\alpha_1 \alpha_2 \cdots \alpha_N\rangle = \psi_{\alpha_1\cdots\alpha_N}(r_1\cdots r_N)$$

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

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

$$\varphi_{\alpha_1}(r_1)\varphi_{\alpha_2}(r_2)\cdots\varphi_{\alpha_N}(r_N)$$

If $\alpha_2$ from $\psi(r_1)$ and $\alpha_1$ from $\psi(r_2)$

$$-\varphi_{\alpha_1}(r_2)\varphi_{\alpha_1}(r_1)\cdots\varphi_N(r_N)$$

$\Rightarrow$ determinant

## 87.3 One-body operators

Diagonal basis:

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

In general: N.B. indep. of # of particles

$$\sum_i U_{\alpha_i}\hat{n}_{\alpha_i} = \sum_i a^+_{\alpha_i}\langle\alpha_i|\hat{U}|\alpha_i\rangle a_{\alpha_i}$$

Change of basis:

$$= \sum_{m,n} a^+_{\mu_m}\langle\mu_m|\hat{U}|\mu_n\rangle a_{\mu_n}$$

Eigenstates:

$$a^+_{\alpha_1} a^+_{\alpha_4}|0\rangle \Rightarrow \text{Slater determinants}$$

In the continuum:

$$\hat{V} = \int d^3r \; V(r)\,\Psi^+(r)\Psi(r)$$

$$\hat{T} = \int\frac{d^3p}{(2\pi)^3}\left(-\frac{\hbar^2}{2m}\right)c^+(p)\;p^2 c(p)$$

## 87.4 Two-body operator

Diagonal basis

$$= \frac{1}{2}\sum_{ij}\langle\alpha_i|\langle\alpha_j|\hat{V}|\alpha_i\rangle|\alpha_j\rangle$$

$$(\hat{n}_{\alpha_i}\hat{n}_{\alpha_j} - \delta_{ij}\hat{n}_{\alpha_i})$$

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

$$\boxed{\hat{V}_{\text{coulomb}} = \frac{1}{2}\sum_{\sigma\sigma'}\int d^3r\,d^3r'\,v(r-r')\,\Psi^+_\sigma(r)\,\Psi^+_{\sigma'}(r')\,\Psi_{\sigma'}(r')\,\Psi_\sigma(r)}$$

# Cours #2 (45 minutes)

## Hubbard model, Green functions Summary

### 82.1 Hubbard model

$$H = -\sum_{ij\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

### 83 Perturbation theory

$$e^{-\beta \hat{K}} = e^{-\beta K_0} \hat{U}(\beta)$$

$$\hat{U}(\beta) \equiv T_\tau \left[ e^{-\int_0^\beta \hat{K}_1(\tau) d\tau} \right]$$

$$\hat{K}_1(\tau) = e^{\hat{K}_0 \tau} K_1 e^{-\hat{K}_0 \tau}$$

### 84 Green functions, useful information

#### 84.1 Photoemission + fermion correlation

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

#### 84.2 Def. Matsubara Green function

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

#### 84.3 Matsubara frequency representation

$$\mathcal{G}_{\alpha\beta}(ik_n) = \int_0^\beta d\tau \, e^{ik_n \tau} \mathcal{G}_{\alpha\beta}(\tau)$$

#### 84.5 Green function at U = 0

$$\mathcal{G}_{k}(ik_n) = \frac{1}{ik_n - \zeta_k}$$

## 82.1 Hubbard model

For solid $\psi^\dagger_\sigma(r) = \sum_{n \atop \sigma} \sum_{R_i} c^\dagger_{in\sigma} \; w^*_n(\vec{r} - \vec{R}_i)$

$$\int d^3r \; w_n(\vec{r} - \vec{R}_i) w_m(\vec{r} - \vec{R}_j) = \delta_{m,n} \, \delta_{R_i, R_j}$$

One band:

$$\hat{T} = \int d^3r \left(\frac{-\hbar^2}{2m}\right) \sum_{R_i} \sum_{R_j \atop \sigma} c^\dagger_{i\sigma} \, w^*_n(\vec{r} - \vec{R}_i) \underline{\nabla}^2 w_m(\vec{r} - \vec{R}_j) \, c_{j\sigma}$$

$$= \sum_{R_i R_j \atop \sigma} c^\dagger_{i\sigma} \langle i | \frac{p^2}{2m} | j \rangle c_{j\sigma} = \sum_{ij} t_{ij} c^\dagger_{i\sigma} c_{j\sigma}$$

Similarly:

$$\hat{V} = \frac{1}{2} \sum_{\sigma\sigma'} \sum_{ijkl} \langle i | \langle j | \hat{V} | k \rangle | l \rangle \; c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{l\sigma'} c_{k\sigma'}$$

Same site only

$$\hat{V} = \frac{1}{2} \sum_{\sigma\sigma'} \sum_i U c^\dagger_{i\sigma} c^\dagger_{i\sigma'} c_{i\sigma'} c_{i\sigma}$$

$$= \sum_i U n_{i\uparrow} n_{i\downarrow}$$

Ground state

$t = 0 \quad |\psi\rangle_{t=0} = \prod_{i\sigma_i} c^\dagger_{i\sigma_i} |0\rangle$ Highly degenerate

$U = 0 \quad |\psi\rangle_{U=0} = \prod_k^{k_F} c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} |0\rangle$

General case:

$|\psi\rangle_{t=0}$ not eigenstate of $\hat{T}$

$|\psi\rangle_{U=0}$ not eigenstate of $\hat{V}$

$|\psi\rangle$ = linear combination

= "quantum fluctuations"

$\Rightarrow$ Mott transition

$\Rightarrow$ Magnetic states (AFM)

d-wave superconductivity

## 83. Perturbation theory and time-ordered product.

$$e^{-\beta(\hat{H}_0+\hat{H}_1-\mu\hat{N})} = e^{-\beta(\hat{K}_0+\hat{K}_1)} = e^{-\beta\hat{K}}$$

$$[\hat{H}_0-\mu_0\hat{N},\ \hat{H}_1] \neq 0 \qquad \hat{K}_0 = \hat{H}_0-\mu\hat{N}$$

$$\boxed{\begin{aligned} e^{-\beta\hat{K}} &= e^{-\beta\hat{K}_0}\,\hat{U}(\beta)\\ \hat{U}(\beta) &= T_\tau\left[e^{-\int_0^\beta d\tau\,\hat{K}_1(\tau)}\right]\\ \hat{K}_1(\tau) &= e^{K_0\tau}K_1e^{-K_0\tau}\end{aligned}}$$

Proof:

$$\frac{\partial}{\partial\tau}\left[e^{-\tau K_0}\hat{U}(\tau)\right] = -(\hat{K}_0+\hat{K}_1)e^{-\tau\hat{K}}$$

$$e^{-\tau K_0}\left[\cancel{-\hat{K}_0\hat{U}(\tau)}+\frac{\partial\hat{U}}{\partial\tau}\right] = -(\cancel{\hat{K}_0}+\hat{K}_1)e^{-\tau\hat{K}_0}U(\tau)$$

$$\frac{\partial\hat{U}(\tau)}{\partial\tau} = -\hat{K}_1(\tau)\hat{U}(\tau)$$

$$\hat{U}(\beta)-\hat{U}(0) = -\int_0^\beta d\tau\,\hat{K}_1(\tau)\hat{U}(\tau)$$

$$\hat{U}(\beta) = 1-\int_0^\beta d\tau\,\hat{K}_1(\tau)+\int_0^\beta d\tau\int_0^\tau d\tau'\,\hat{K}_1(\tau)\hat{K}_1(\tau')$$

$$-\int_0^\beta d\tau\int_0^\tau d\tau'\int_0^{\tau'} d\tau''\,\hat{K}_1(\tau)\hat{K}_1(\tau')\hat{K}_1(\tau'')+\cdots$$

Recover exponential by defining $T_\tau$ time ordering and allowing $n!$ permutations.

## Non equilibrium

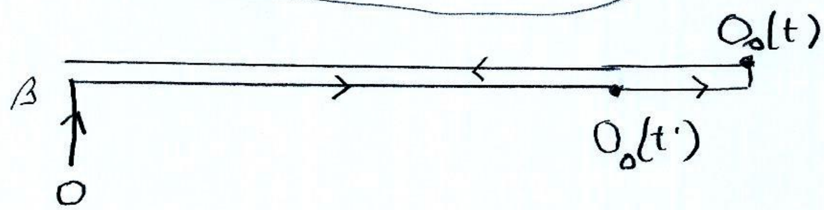
$$\frac{1}{Z} \mathrm{Tr}\left[ e^{-\beta(K_0+K_1)} e^{iHt/\hbar} O e^{-iHt/\hbar} e^{iHt'/\hbar} O' e^{-iHt'/\hbar} \right]$$

$$= \frac{1}{Z} \mathrm{Tr}\left[ e^{-\beta K_0} U(\beta,0) U(0,it)\, O_0(t)\, U(it,0) \right.$$

$$\left. U(0,it')\, O_0'(t')\, U(it',0) \right]$$

$$\boxed{\begin{array}{l} it = \tau \\ t = -i\tau \end{array}}$$

$$e^{-iHt} = e^{-iH_0 t}\, U(it,0)$$




$$O_0(t) = e^{iHt}\, O\, e^{-iHt}$$

# Cours #3 (90 min) 7 juin 2022

## Spectral weigth, self-energy Summary

84.4 Spectral weight, relation to $\mathcal{G}_k(ik_n)$ and $\frac{\partial^2\sigma}{\partial\Omega\partial\omega}$

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

84.6 Spectral weight from $\mathcal{G}_k(ik_n)$ analytic continuation.

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

$$G^R_k(\omega) = \int \frac{d\omega'}{2\pi} \frac{A_k(\omega')}{\omega+i\eta-\omega'}$$

85. Self-energy and the effect of interactions

85.1 The atomic limit $t=0$

$$G^R_{k\uparrow} = \frac{1-\langle n_\downarrow\rangle}{\omega+i\eta+\mu} + \frac{\langle n_\downarrow\rangle}{\omega+i\eta+\mu-U}$$

85.2 self-energy, atomic limit (Mott insulators)

Dyson's equation

$$G^R_{k\uparrow}(\omega)^{-1} = G^{(0)R}_{k\uparrow}(\omega)^{-1} - \Sigma^R_{k\uparrow}(\omega)$$

85.3 Properties.

$$\mathrm{Im}\,\Sigma^R_{k\uparrow} < 0$$

85.4 Anderson impurity problem, hybridization

$$G^R_\uparrow(\omega)^{-1} = G^{(0)R}_\uparrow(\omega)^{-1} - \Delta^R_\uparrow(\omega) - \Sigma^R_\uparrow(\omega)$$

## 84.4 Spectral weight and relation to photoemission

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

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

Lehmann representation

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

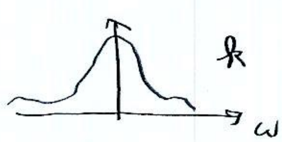
$A_k(\omega)$ = spectral weight

$$\boxed{A_k(\omega) = 2\pi \sum_{n,m} \frac{e^{-\beta K_m}}{Z} \left(1+e^{\beta\omega}\right) \left|\langle n| c_k |m\rangle\right|^2 \delta(\omega-(K_m-K_n))}$$

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

Spectral weight is normalized

$$\int \frac{d\omega}{2\pi} A(k,\omega) = \sum_{m,n} \left(e^{-\beta K_m} + e^{-\beta K_n}\right) \frac{1}{Z} \langle n| c_k^\dagger |m\rangle \langle m| c_k |n\rangle$$




$$= \langle \{ c_k, c_k^\dagger \} \rangle = 1$$

Free particle: n, m eigenstates with $c_k$ ⇒

$$A_k(\omega) = 2\pi\,\delta(\omega-\xi_k)\ ; \quad \mathcal{G}_k(\omega) = \frac{1}{ik_n-\xi_k}$$

## 84.6 $A_k(\omega)$ from $\mathcal{G}$ : analytic continuation

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

$$G^R(\omega) = \mathcal{G}(ik_n \to \omega + i\eta)$$

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

# 85 Self-energy and the effects of interactions

## 85.1 The atomic limit

$$\hat{K} = \sum_i U n_{i\uparrow} n_{i\downarrow} - \mu n_{i\uparrow} - \mu n_{i\downarrow}$$

$$Z = 1 + 2e^{\beta\mu} + e^{2\beta\mu - \beta U}$$

$$\langle n_\uparrow \rangle = \frac{e^{\beta\mu} + e^{2\beta\mu-\beta U}}{Z} = \frac{Z - e^{\beta\mu} - 1}{Z} = 1 - \frac{e^{\beta\mu}+1}{Z}$$

$$\mathcal{G}_{k\uparrow}(\tau) \underset{\tau>0}{=} -\langle c_\uparrow(\tau) c_\uparrow^+ \rangle$$

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

$$- \frac{1}{Z} e^{\beta\mu} \langle \uparrow | e^{K\tau} c_\uparrow e^{-K\tau} | \uparrow\downarrow \rangle \langle \uparrow\downarrow | c^+_{k\uparrow} | 0 \rangle$$

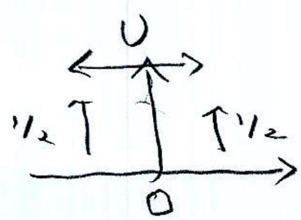
$$= -\frac{e^{\mu\tau}}{Z} - \frac{1}{Z} e^{\beta\mu} \left[ e^{-\mu\tau} e^{2\mu\tau - U\tau} \right]$$

$$\int_0^\beta d\tau\, e^{ik_n\tau} \mathcal{G}_{k\uparrow}(\tau) = \mathcal{G}_{k\uparrow}(ik_n)$$

$$= -\frac{1}{Z} \frac{e^{(ik_n+\mu)\beta} - 1}{ik_n+\mu} - \frac{1}{Z} e^{\beta\mu} \frac{\left[ e^{(ik_n+\mu-U)\beta} - 1 \right]}{ik_n+\mu-U}$$

$$= \frac{1}{Z} \frac{e^{\beta\mu}+1}{ik_n+\mu} + \frac{e^{2\beta\mu-\beta U} + e^{\beta\mu}}{ik_n+\mu-U}$$

$$= \frac{1-\langle n_\uparrow \rangle}{ik_n+\mu} + \frac{\langle n_\uparrow \rangle}{ik_n+\mu-U}$$




$\mu = \frac{U}{2}$

- normalized
- indep. of $\vec{k}$

## 85.2 Self-energy

For the general case we define the self-energy by

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

Effect of interactions

Why? Because natural interpretation as lifetime

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

### Dyson's equation

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

Hence

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

or

$$G^R_{k\sigma}(\omega) = G^{R(0)}_{k\sigma}(\omega) + G^{R(0)}_{k\sigma}(\omega)\, \Sigma^R_{k\sigma}(\omega)\, G^R_{k\sigma}(\omega)$$

## 85.3 A few properties

$\operatorname{Im}\Sigma^R_{k\sigma}(\omega) < 0$ for causality
Poles in l.h.p.

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

## 83.4 Integrating out the bath: Anderson impurity

$$\hat{K}_I = H_f + H_c + H_{fc} - \mu N$$

$$\underset{\underset{-f_\sigma}{\updownarrow V_{k0}}}{\overset{0}{-}}$$

① $K_f = \sum_\sigma (\epsilon - \mu) f^+_\sigma f_\sigma + U \left( f^+_\uparrow f_\uparrow \right) \left( f^+_\downarrow f_\downarrow \right)$ (Impurity)

② $K_c = \sum_{\sigma k} (\epsilon_k - \mu) c^+_{k\sigma} c_{k\sigma}$ (conduction)

③ $K_{fc} = \sum_\sigma \sum_k \left( V_{k0} c^+_{k\sigma} f_\sigma + V^*_{0k} f^+_\sigma c_{k\sigma} \right)$ (Hybridation)

**Note:** $U \left[ f^+_\downarrow f_\downarrow f^+_\uparrow f_\uparrow , f_\sigma \right] = - f_\sigma$

since $[n_{\sigma'}, f_\sigma] = - f_\sigma \delta_{\sigma\sigma'}$

---

(1) $\frac{\partial}{\partial \tau} \mathcal{G}_{ff\sigma}(\tau) = -\delta(\tau) - (\epsilon - \mu) \mathcal{G}_{ff\sigma}(\tau) \underset{\uparrow}{-} \sum_k V^*_{0k} \mathcal{G}_{cf}(k;\tau)$

anticomm. avec $c_{k\sigma}$

$+ U \langle T_\tau f^+_\downarrow(\tau) f_\downarrow(\tau) f_\uparrow(\tau) f^+_\uparrow(0) \rangle$

(2) $\frac{\partial}{\partial \tau} \mathcal{G}_{cf\sigma}(k;\tau) = -(\epsilon_k - \mu) \mathcal{G}_{cf\sigma}(k;\tau) - V_{k0} \mathcal{G}_{ff}(\tau)$

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

In Matsubara (2) → (1) gives

$$\boxed{\left[ ik_n - (\epsilon - \mu) - \sum_k V^*_{0k} \frac{1}{ik_n - (\epsilon_k - \mu)} V_{k0} - \Sigma_{ff\sigma}(ik_n) \right] \mathcal{G}_{ff\sigma}(ik_n) = 1}$$

$$\equiv \Delta(ik_n)$$

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As if time-dependent non-interacting Hamiltonian

Action formalism more suited

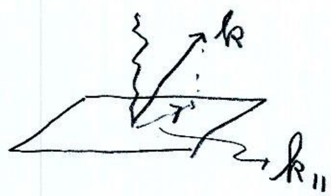
Note: Interpretation as sum over all trajectories

Note: Matrix structure below

$$\begin{bmatrix} ik_n-(\epsilon-\mu)-\Sigma_{ff\sigma}(ik_n) & -V^*_{0k_0} & -V^*_{0k_1} & \cdots \\ -V_{k_0 0} & ik_n-(\epsilon_{k_0}-\mu) & 0 & \\ -V_{k_1 0} & 0 & ik_n-(\epsilon_{k_1}-\mu) & \\ \vdots & & & \end{bmatrix} \begin{bmatrix} \mathcal{G}_{ff\sigma}(ik_n) \\ \mathcal{G}_{c0\sigma}(k_0, ik_n) \\ \mathcal{G}_{c0\sigma}(k_1, ik_n) \\ \vdots \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}$$

# 84 Green functions : necessary and useful

## 84.1 Photoemission and fermion correlations




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

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

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

$$A_q \propto (a_q + a^+_{-q}) \quad q \to 0$$

$$j_{q=0} \propto \sum_p \frac{\vec{p}}{m} c^+_p c_p$$

$$\boxed{\frac{\partial^2 \sigma}{\partial\Omega\,\partial\omega} \propto \text{Known Matrix Elements} \times \frac{2\pi}{\hbar} \sum_{m,n} \frac{e^{-\beta K_m}}{Z} \langle m| c^+_{k_\parallel} |n\rangle \langle n| c_{k_\parallel} |m\rangle \,\delta\left(\hbar\omega - (K_m - K_n)\right)}$$

## 84.2 Definition of $\mathcal{G}$

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

$$\equiv -\langle c_\alpha(\tau) c^+_\beta(0)\rangle \Theta(\tau) + \langle c^+_\beta(0) c_\alpha(\tau)\rangle \Theta(-\tau)$$

Note: $T_\tau$ motivated by perturbation theory

$$\langle O\rangle = \mathrm{Tr}\,[\rho\, O]$$

$$c_\alpha(\tau) = e^{\hat{K}\tau} c_\alpha e^{-\hat{K}\tau}$$

$$c^+_\alpha(\tau) = e^{\hat{K}\tau} c^+_\alpha e^{-\hat{K}\tau}$$

Note: $\hbar = 1$ $\quad c^+_\alpha(\tau)$ not adjoint of $c(\tau)$

## 84.3 Matsubara frequencies

Antiperiodicity: $\mathcal{G}_{\alpha\beta}(\tau) = -\mathcal{G}_{\alpha\beta}(\tau-\beta) \quad \tau > 0$

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

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

Fourier series $\Rightarrow$

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

6 juin 2022 (B)

# 84.5 $\mathcal{G}(ik_n)$ for $U=0$

$$\hat{K}_0 = \sum_p \xi_p c_p^+ c_p \quad \text{(drop spin)}$$

$$\frac{\partial \mathcal{G}_k(\tau)}{\partial \tau} = \frac{\partial}{\partial \tau}\left[ - \langle T_\tau c_k(\tau) c_k^+(0) \rangle \right)$$

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

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

since $\frac{\partial c_k(\tau)}{\partial \tau} = [\hat{K}_0, c_k] = -\xi_k c_k(\tau)$

$$\int_{0^+}^{\beta} d\tau \, e^{ik_n \tau} \frac{\partial}{\partial \tau} \mathcal{G}_k(\tau) = -\xi_k \mathcal{G}_k(ik_n)$$

$$\left[ e^{ik_n \tau} \mathcal{G}_k(\tau) \right|_{0^+}^{\beta} - ik_n \mathcal{G}_k(ik_n) = -\xi_k \mathcal{G}_k(ik_n)$$

$$-\mathcal{G}_k(\beta) - \mathcal{G}_k(0^+) = (ik_n - \xi_k)\mathcal{G}(ik_n)$$

$$\mathcal{G}_k(0^+) \to \langle c_k c_k^+ \rangle$$

$$\mathcal{G}_k(\beta) \to \frac{1}{Z} \mathrm{Tr}\left[ e^{-\beta \hat{K}_0} e^{\beta \hat{K}_0} c_k e^{-\beta \hat{K}_0} c_k^+ \right] = \langle c_k^+ c_k \rangle$$

cyclic.

$$\langle c_k c_k^+ \rangle + \langle c_k^+ c_k \rangle = 1$$

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

7 juin 2022 (21)

# 79. Coherent states for fermions

Cours #4

Summary

## 79.1 Grassmann variables for fermions

$$c|\eta\rangle = \eta|\eta\rangle \quad ; \quad |\eta\rangle = e^{-\eta c^+}|0\rangle$$

## 79.2 Grassmann integrals

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

## 79.3 Change of variables

$$\psi_i = \sum_{j=1}^{N} U_{ij}\eta_j \; ; \; \prod_{i=1}^{N}\int d\psi_i = \det[U]\prod_{k=1}^{N}\int d\eta_k$$

## 79.4 Grassmann Gaussian integrals

$$\int \mathcal{D}\eta^+ \int \mathcal{D}\eta\, e^{-\eta^+ A\eta - \eta^+ J - J^+\eta} = \det[A]\, e^{J^+ A^{-1} J}$$

## 79.5 Closure, overcompleteness, trace formula

$$\mathrm{Tr}[O] = \int d\eta^+ \int d\eta\, e^{-\eta^+\eta}\langle -\eta|O|\eta\rangle$$

## 80.1 + 80.2 Single fermions

$$Z = \int \mathcal{D}\eta^+ \int \mathcal{D}\eta\, e^{-S}$$

$$S = \int_0^\beta d\tau \left(\eta^+(\tau)\frac{\partial}{\partial\tau}\eta(\tau) + \epsilon(\tau)\eta^+(\tau)\eta(\tau)\right)$$

## 80.3 Wick's theorem

$$(-1)^n \langle T_\tau c(\tau_n) c^+(\tau'_n) \cdots c(\tau_2)c^+(\tau'_2)\, c(\tau_1) c^+(\tau'_1)\rangle$$

$$= (-1)^n \frac{1}{Z}\int \mathcal{D}\eta^+ \int \mathcal{D}\eta\, e^{-\eta^+\mathcal{G}^{-1}\eta}\, \eta(\tau_n)\eta^+(\tau'_n) \cdots \eta(\tau_2)\eta^+(\tau'_2)\,\eta(\tau_1)\eta^+(\tau'_1)$$

$$= \det\begin{bmatrix} \mathcal{G}(\tau_1,\tau'_1) & \mathcal{G}(\tau_1,\tau'_2) & \cdots & \mathcal{G}(\tau_1,\tau'_n) \\ \mathcal{G}(\tau_2,\tau'_1) & \mathcal{G}(\tau_2,\tau'_2) & \cdots & \mathcal{G}(\tau_2,\tau'_n) \\ \vdots & & & \\ \mathcal{G}(\tau_n,\tau'_1) & \mathcal{G}(\tau_n,\tau'_2) & \cdots & \mathcal{G}(\tau_n,\tau'_n) \end{bmatrix}$$

## 80.5 Quant. Imp.

$$\Delta(ik_n) = \sum_k \frac{V^*_{ik} V_{ki}}{ik_n - \xi_k}$$

# 79. Coherent states for fermions

## 79.1 Grassmann variables for fermions

$c|\eta\rangle = \eta|\eta\rangle$ analogy with bosons

Eigenvalues = numbers that anticommute.

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

$\eta_1 \eta_2 |\eta_1 \eta_2\rangle = -\eta_2 \eta_1 |\eta_1 \eta_2\rangle$

$\{\eta_1, \eta_1^+\} = 0$ inside Tr

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

$$c|\eta\rangle = c|0\rangle + \eta c c^+|0\rangle \qquad \{\eta, c\} = 0$$

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

$$= \eta|\eta\rangle$$

## 79.2 Grassman integrals

All functions first order in $\eta$

$$\int d\eta = 0 \Rightarrow \int d\eta\, f(\eta + \xi) = \int d\eta\, f(\eta)$$

$$\int d\eta\, \frac{\partial f}{\partial \eta} = 0$$

$$\int d\eta\, \eta = 1 \Rightarrow \int d\eta\, (a f(\eta) + b g(\eta))$$

$$= \int d\eta\, a f(\eta) + \int d\eta\, b g(\eta)$$

product of 2 Grassmann numbers is an ordinary number

## 79.3 Change of variables

$$\psi_i = \sum_{j=1}^{N} U_{ij}\,\eta_j$$

$$\underbrace{\int d\psi_1 \cdots d\psi_N}_{\mathcal{D}\psi} = \sum_{j_1=1}^{N} \cdots \sum_{j_N=1}^{N} U_{1j_1} U_{2j_2} \cdots U_{Nj_N} \int d\eta_{j_1} d\eta_{j_2} \cdots d\eta_{j_N}$$

$$= \sum_{j_1=1}^{N} \cdots \sum_{j_N=1}^{N} U_{1j_1} U_{2j_2} \cdots U_{Nj_N}\, \epsilon^{j_1 j_2 \cdots j_N} \underbrace{\int d\eta_1\, d\eta_2 \cdots d\eta_N}_{\mathcal{D}\eta}$$

$$= \det[U] \int d\eta_1 \cdots d\eta_N$$

Short-cut

## 79.4 Grassmann Gaussian integrals

$$\int d\eta^+ \int d\eta\; e^{-\eta^+ a \eta} = \int d\eta^+ \int d\eta\, (1 - \eta^+ a \eta) = a$$

$$= e^{\ln a}$$

$$\int d\eta_1^+ \int d\eta_1 \int d\eta_2^+ \int d\eta_2\; e^{-\eta_1^+ a_1 \eta_1 - \eta_2^+ a_2 \eta_2}$$

$$= a_1 a_2 = e^{\ln a_1 + \ln a_2}$$

$$\boxed{\int \mathcal{D}\eta^+ \int \mathcal{D}\eta\; e^{-\eta^+ A \eta} = \det[A] = \exp[\operatorname{Tr} \ln A]}$$

Source field ($J$ is a Grassman variable)

$$\int d\eta^+ \int d\eta\; e^{-\eta^+ a \eta - \eta^+ J - J^+ \eta}$$

$$= \int d\eta^+ \int d\eta\; e^{-(\eta^+ + J^+ a^{-1})\, a\, (\eta + a^{-1} J) + J^+ a^{-1} J}$$

$$= a\, e^{J^+ a^{-1} J}$$

## 79.5 Closure, overcompleteness Trace formula

$$\int d\eta^+ \int d\eta \; e^{-\eta^+\eta} \; |\eta\rangle\langle\eta|$$

$$= \int d\eta^+ \int d\eta \; (1-\eta^+\eta)(1-\eta c^+)|0\rangle\langle 0|(1-c\eta^+)$$

odd # of $\eta \Rightarrow 0$

$$= \underset{(1)}{|0\rangle\langle 0|} + \underset{(2)}{|1\rangle\langle 1|} = \mathbb{1}$$

### Over completeness

$$\langle \eta_1 | \eta_2 \rangle = \langle 0|(1-c\eta_1^+)(1-\eta_2 c^+)|0\rangle$$

$$= \langle 0|0\rangle + \eta_1^+\eta_2 \langle 1|1\rangle$$

$$= e^{\eta_1^+\eta_2}$$

### Trace

$$\mathrm{Tr}[O] = \int d\eta^+ \int d\eta \; e^{-\eta^+\eta} \langle -\eta | O | \eta\rangle$$

$$= \int d\eta^+ \int d\eta \; (1-\eta^+\eta) \langle 0|(1+c\eta^+) O (1-\eta c^+)|0\rangle$$

$$= \underset{(1)}{\langle 0|O|0\rangle} + \underset{(2)}{\langle 1|O|1\rangle}$$

# 80. Coherent state functional integral for fermions

## 80.1 Simple example single fermions

Trotter $e^{-\beta(\hat{T}+\hat{V})} = \prod_{i=1}^{N_\tau} e^{-\Delta\tau \hat{T}} e^{-\Delta\tau \hat{V}}$

Closure

Trace

$$\int d\eta^+ \int d\eta \, e^{-\eta^+\eta} |\eta\rangle\langle\eta|$$

$$\boxed{Z = \int \mathcal{D}\eta^+ \int \mathcal{D}\eta \, e^{-S}}$$

From closure

$$\boxed{S = \int_0^\beta d\tau \left( \eta^+(\tau) \frac{\partial}{\partial\tau} \eta(\tau) + \hat{H}(\eta^+, \eta) \right)}$$

$$\eta^+ = \frac{\partial L}{\partial \mathring{\eta}} \leftrightarrow p = \frac{\partial L}{\partial \mathring{q}} \qquad L = p\mathring{q} - H$$

Start from final result in the diagonal basis,

then

$$\mathcal{G} = - \frac{\int d\eta^+ \int d\eta \, e^{-\eta^+(-\mathcal{G}^{-1})\eta} \eta \eta^+}{\int d\eta^+ \int d\eta \, e^{-\eta^+(-\mathcal{G}^{-1})\eta}} = \frac{-1}{(-\mathcal{G}^{-1})}$$

$$\boxed{S = \sum_{n=-\infty}^{\infty} \eta_n^+ (-ik_n + \epsilon) \eta_n}$$

## 80.3 Wick's theorem

$$\frac{(-1)^m \int \mathcal{D}\eta^+ \int \mathcal{D}\eta \, e^{-\eta^+(-\mathcal{G}^{-1})\eta} \eta_1\eta_1^+ \eta_2\eta_2^+ \cdots \eta_m\eta_m^+}{\int \mathcal{D}\eta^+ \int \mathcal{D}\eta \, e^{-\eta^+(-\mathcal{G}^{-1})\eta}}$$

$$= \mathcal{G}_{11}\mathcal{G}_{22}\mathcal{G}_{33}\cdots\mathcal{G}_{mm}$$

This is the det of a matrix

$$(-1)^m \langle c(\tau_m)c^+(\tau_m') \cdots c(\tau_2)c^+(\tau_2')c(\tau_1)c^+(\tau_1')\rangle$$

$$= (-1)^m \frac{1}{Z} \int \mathcal{D}\eta^+ \int \mathcal{D}\eta \, e^{-\eta^+(-\mathcal{G}^{-1})\eta} \eta(\tau_m)\eta^+(\tau_m') \cdots \eta(\tau_1)\eta^+(\tau_1')$$

$$= \det \begin{bmatrix} \mathcal{G}(\tau_1,\tau_1') & \mathcal{G}(\tau_1,\tau_2') & \cdots & \mathcal{G}(\tau_1,\tau_m') \\ \mathcal{G}(\tau_2,\tau_1') & \mathcal{G}(\tau_2,\tau_2') & \cdots & \mathcal{G}(\tau_2,\tau_m') \\ \vdots & & & \\ \mathcal{G}(\tau_m,\tau_1') & \mathcal{G}(\tau_m,\tau_2') & \cdots & \mathcal{G}(\tau_m,\tau_m') \end{bmatrix}$$

means perturbation theory in powers of interaction, same structure, whatever frequency dependence of $\mathcal{G}$.

# 80.5 Effective action for quantum impurity

$f \to \Psi \qquad c \to \eta$

$$Z = \int \mathcal{D}\Psi^+ \int \mathcal{D}\Psi \int \mathcal{D}\eta^+ \int \mathcal{D}\eta \, e^{-(S_I + S_b + S_{Ib})}$$

$$S_{Ib} = \int_0^\beta d\tau \sum_k \sum_\sigma \left[ V_{ik}^* \Psi_\sigma^+(\tau) \eta_\sigma(k,\tau) + V_{ki} \underbrace{\eta_\sigma^+(k,\tau) \Psi_\sigma(\tau)}_{} \right]$$

$$J_\sigma(k,\tau) = V_{ki} \Psi_\sigma(\tau)$$

We can integrate over the bath since it is quadratic.

$$\boxed{Z = e^{\mathrm{Tr} \ln(-\mathcal{G}_b^{-1})} \int \mathcal{D}\Psi^+ \mathcal{D}\Psi \, e^{-S_I + J^+ (-\mathcal{G}_b^{-1})^{-1} J}}$$

Drops from observables

In diagonal basis

$$J^+(-\mathcal{G}_b) J = \sum_{n\sigma} \Psi_\sigma^+(ik_n) \left( \sum_k V_{ik}^* \frac{-1}{ik_n - (\epsilon_k - \mu)} V_{ki} \right) \Psi_\sigma(ik_n)$$

$$= - \sum_{n\sigma} \Psi_\sigma^+(ik_n) \Delta_\sigma(ik_n) \Psi_\sigma(ik_n)$$

Hence

$$\boxed{\mathcal{G}^{0\,-1}(ik_n) = ik_n - (\epsilon - \mu) - \Delta(ik_n)}$$

## Hybridization expansion

Take 2 Matsubara frequencies (diag. basis) to illustrate.

$$Z = C \int d\psi_1^+ \int d\psi_1 \int d\psi_2^+ \int d\psi_2 \, e^{-S_F} \, [\underbrace{(1-\psi_1^+\Delta_1\psi_1)(1-\psi_2^+\Delta_2\psi_2)}_{\mathcal{A}}]$$

$$\mathcal{A} = (1 - \underbrace{\psi_1^+\Delta_1\psi_1 - \psi_2^+\Delta_2\psi_2} + \psi_1^+\Delta_1\psi_1\psi_2^+\Delta_2\psi_2)$$

In the end will give sum over all Matsubara freq.

$$-T\sum_{n=-\infty}^{\infty} \int_0^\beta d\tau_1' \, e^{-ik_n\tau_1'} \psi^+(\tau_1') \int_0^\beta d\tau'' e^{ik_n\tau''} \Delta(\tau'') \int_0^\beta d\tau_1 \, e^{ik_n\tau_1} \psi(\tau_1)$$

N.B $\Delta$ is scalar, commutes with $\psi$

$$= \int_0^\beta d\tau_1' \int_0^\beta d\tau_1 \, \psi^+(\tau_1') \, \Delta(\tau_1'-\tau_1) \, \psi(\tau_1)$$

In higher order when we go to $\psi(\tau)$, any given $\psi^{(+)}(\tau)$ must occur only once in a product.

But in imaginary time a given $\psi(\tau_i)$ may come from $\psi_1$ or from $\psi_2$. Similarly for $\psi^+(\tau_i)$

Reordering to always get the same time order and taking care of anticommutation will yield the determinant of $\Delta$

Finally evaluating the final expression in the canonical formalism

$$Z = C \sum_{k=0}^{\infty} (-1)^k \int_0^\beta d\tau_1' \int_{\tau_1'}^\beta d\tau_2' \cdots \int_{\tau_{k-1}'}^\beta d\tau_k' \int_0^\beta d\tau_1 \int_{\tau_1}^\beta d\tau_2 \cdots \int_{\tau_{k-1}}^\beta d\tau_k$$

$$\langle T_\tau f^+(\tau_k') f(\tau_k) f^+(\tau_{k-1}') f(\tau_{k-1}) \cdots f^+(\tau_1') f(\tau_1) \rangle_{H_I}$$

$$\det \begin{bmatrix} \Delta(\tau_1'-\tau_1) & \Delta(\tau_1'-\tau_2) & \cdots & \Delta(\tau_1'-\tau_k) \\ \Delta(\tau_2'-\tau_1) & \Delta(\tau_2'-\tau_2) & \cdots & \Delta(\tau_2'-\tau_k) \\ \vdots & & & \\ \Delta(\tau_k'-\tau_1) & \Delta(\tau_k'-\tau_2) & \cdots & \Delta(\tau_k'-\tau_k) \end{bmatrix}$$

8 juin 2022 (29)

# Many-body perturbation theory
## Source fields, Luttinger Ward,

(90 minutes)

Summary

Cours #5

## 87 Source fields for Many-body Green's function.

### 87.1 A simple example in classical stat. mech.

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

### 87.2 Green's functions and higher order correlation functions.

$$Z[\varphi] = \mathrm{Tr}\left[e^{-\beta K} T_\tau\, e^{-\psi^\dagger(\bar 1)\varphi(\bar 1,\bar 2)\psi(\bar 2)}\right] \; ; \; \mathcal{G}(1,2)_\varphi = -\frac{\delta \ln Z[\varphi]}{\delta\varphi(2,1)}$$

## 88. Equations of motion to find $\mathcal{G}(1,2)_\varphi$ and $\Sigma(1,2)_\varphi$

### 88.1 Equation of motion for $\psi(1)$

$$\frac{\partial\psi(1)}{\partial\tau_1} = \frac{\nabla^2}{2m}\psi(1) + \mu\psi(1) - \psi^\dagger(\bar 2)\psi(\bar 2)V(\bar 2-1)\psi(1)$$

### 88.2 Equation of motion for $\mathcal{G}(1,2)_\varphi$ and def. of $\Sigma(1,2)_\varphi$

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

## 72. Luttinger-Ward functional and Legendre transform

72.3 $\Omega[\mathcal{G}] = F[\varphi] - \mathrm{Tr}[\varphi\mathcal{G}]$ ; $\frac{1}{T}\frac{\delta\Omega[\mathcal{G}]}{\delta\mathcal{G}(1,2)} = 0$ in equil.

## 76. Constraining field method

### 76.1 Another derivation of Baym-Kadanoff

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

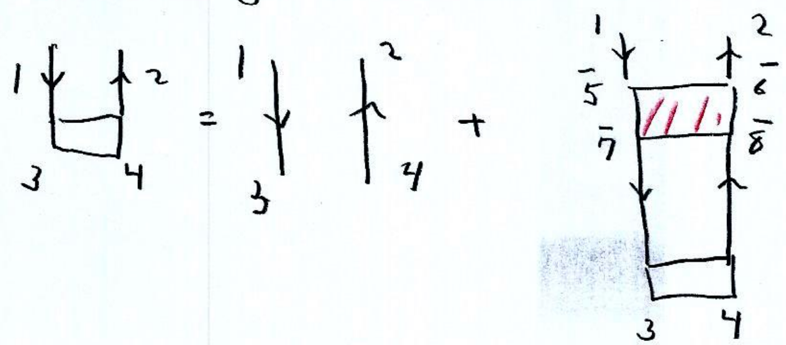
$$\frac{1}{T}\frac{\delta\Phi[\mathcal{G}]}{\delta\mathcal{G}(1,2)} = \Sigma(2,1) \; ; \; \Phi_{\lambda=1}[\mathcal{G}] = \int_0^1 d\lambda\,\frac{1}{\lambda}\langle\lambda\hat V\rangle_\lambda$$

$$\boxed{\Sigma(1,\bar 2)_\varphi\,\mathcal{G}(\bar 2,3)_\varphi = -V(\bar 2-1)\langle T_\tau\,\psi^\dagger(\bar 2^+)\psi(\bar 2)\psi(1)\psi^\dagger(3)\rangle_\varphi}$$

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

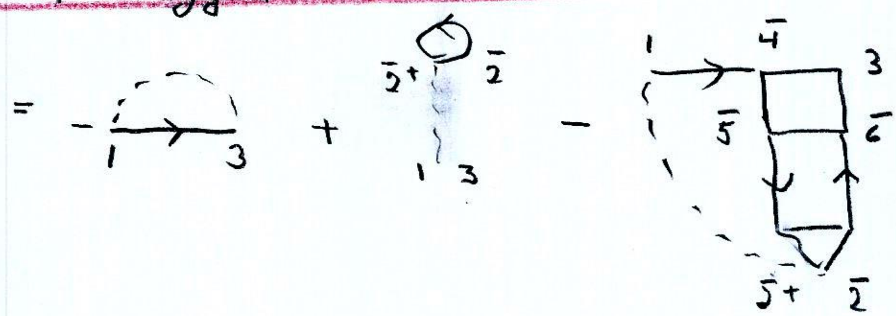
## 36.3 Integral equation for 4-pt function

**Summary**



## 36.4 Self-energy from functional derivative

$\Sigma(1,3) =$



# 87. Source fields for Many-body Green's functions

## 87.1 Simple example from classical stat. mech.

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

Operators that commute

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

$$\frac{\delta h(x)}{\delta h(x')} = \delta(x-x') \quad \text{generalisation of partial derivative}$$

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

From the denominator

In particular works at $h=0$

## 87.2 Green functions and higher order correlation functions

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

$$\psi(1) = \psi_{\sigma_1}(x_1, \tau_1)$$

Overbar, e.g. $\bar{1}$ means $\int d^3x_1 \int_0^\beta d\tau_1 \sum_{\sigma_1}$

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

Under time-ordered product, derivatives as usual

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

$$\equiv \boxed{-\langle T_\tau \psi(1)\psi^\dagger(2)\rangle_\varphi}$$

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

# 88. Equation of motion for $\mathcal{G}_\varphi$ and $\Sigma_\varphi$

## 88.1 Equation of motion for $\psi(1)$

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

N.B.: $[\psi^+(1)\psi(1), \psi(2)] = -\psi(2)\,\delta(1-2)$

$$[AB, C] = ABC + ACB - ACB - CAB = A\{B,C\} - \{A,C\}B$$

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

## 88.2 Equation of motion for $\mathcal{G}_\varphi$ and def. of $\Sigma_\varphi$

$$\frac{\partial}{\partial \tau_1}\mathcal{G}(1,2) = -\delta(\tau_1)\langle\{\psi(r_1,\tau_1), \psi^+(r_2,\tau_1)\}\rangle - \langle T_\tau \frac{\partial \psi(1)}{\partial \tau_1}\psi^+(2)\rangle$$

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

$$\boxed{\begin{aligned} &[\mathcal{G}_0^{-1}(1,\bar{2}) - \varphi(1,\bar{2}) - \Sigma(1,\bar{2})]\,\mathcal{G}(\bar{2},2)_\varphi = \delta(1-2) \\ &\Sigma(1,\bar{2})_\varphi\,\mathcal{G}(\bar{2},2)_\varphi = -\langle T_\tau \psi^+(\bar{2}^+)\psi(\bar{2})V(\bar{2}-1)\psi(1)\psi^+(2)\rangle_\varphi \end{aligned}}$$

$$V(\bar{2}-1) = V(1-\bar{2})$$

# 72 Luttinger-Ward and related functionals

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

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

Prefer to work in terms of observable $\mathcal{G}$ ⇒ Legendre transform based on (1) and (2)

(2) $\boxed{\Omega[\mathcal{G}] = F[\varphi] - \mathrm{Tr}[\mathcal{G}\varphi]}$

Free energy at $\varphi = 0$

Kadanoff-Baym functional (assumes local convexity)

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

$$= T\sum_{ik_n}\sum_{k}\varphi(k,ik_n)\,\mathcal{G}(k,ik_n)$$

Like all Legendre transforms

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

Proof: $\frac{1}{T}\frac{\delta\Omega}{\delta\mathcal{G}} = \left[\cancel{\frac{1}{T}\frac{\delta F[\varphi]}{\delta\varphi}\frac{\delta\varphi}{\delta\mathcal{G}} - \mathcal{G}\frac{\delta\varphi}{\delta\mathcal{G}}} - \varphi\right]$

From equations of motion.

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

Thus have extremum principle

In equilibrium, $\varphi = 0$ and Dyson satified

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# 76. Constraining field method

## 76.1 Another derivation of Baym-Kadanoff

General property of Legendre transforms:

$$dE = TdS - p\,dV \Rightarrow p = -\left(\frac{\partial E}{\partial V}\right)_S$$

$$dF = -SdT - p\,dV \Rightarrow p = -\left(\frac{\partial F}{\partial V}\right)_T$$

Here:

$$\left.\frac{\partial \Omega_{e^2}[\mathcal{G}]}{\partial e^2}\right|_{\mathcal{G}} = \left.\frac{\partial F_{e^2}[\varphi]}{\partial e^2}\right|_{\varphi} = \frac{1}{e^2}\langle \hat{V}\rangle_{e^2}$$

Integrating both sides:

$$\Omega_{e^2}[\mathcal{G}] = \Omega_{e^2=0}[\mathcal{G}] + \int_0^{e^2} d(e'^2)\,\frac{1}{e'^2}\langle \hat{V}\rangle_{e'^2}$$

$$= \left(F_{e^2=0}[\varphi_0] - \mathrm{Tr}[\varphi_0\mathcal{G}]\right) + \Phi_{e^2}[\mathcal{G}]$$

Where

- Constraining field $\varphi_0$ is such that
  $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \varphi_0$ i.e. $\mathcal{G}$ is actual solution
- Luttinger Ward functional

$$\Phi[\mathcal{G}] = \int_0^{e^2} d(e'^2)\,\frac{1}{(e'^2)}\langle \hat{V}\rangle_{e'^2}$$

$$\boxed{\Omega_{e^2}[\mathcal{G}] = \underbrace{\mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_0}\right)\right]}_{F_{e^2}[\varphi_0] \text{ from Grassmann}} - \mathrm{Tr}\left[\underbrace{(\mathcal{G}_0^{-1} - \mathcal{G}^{-1})}_{\varphi_0}\mathcal{G}\right] + \Phi_{e^2}[\mathcal{G}]}$$

$$\boxed{\frac{\delta\Omega_{e^2}}{\delta\mathcal{G}} = -\varphi = \mathcal{G}^{-1} - \mathcal{G}_0^{-1} + \frac{\delta\Phi_{e^2}[\mathcal{G}]}{\delta\mathcal{G}}} \quad \boxed{\Rightarrow \Sigma_{\varphi}[\mathcal{G}] = \frac{\delta\Phi_{e^2}[\mathcal{G}]}{\delta\mathcal{G}}}$$

## 36. Equation of motion for $\mathcal{G}$ in the presence of source fields
## The general many-body problem

### 36.3 An integral equation for the 4-point function

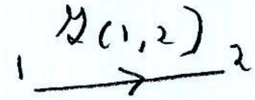
$$\frac{\delta}{\delta \varphi}\left(\mathcal{G}^{-1}\mathcal{G}\right) = 0$$

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

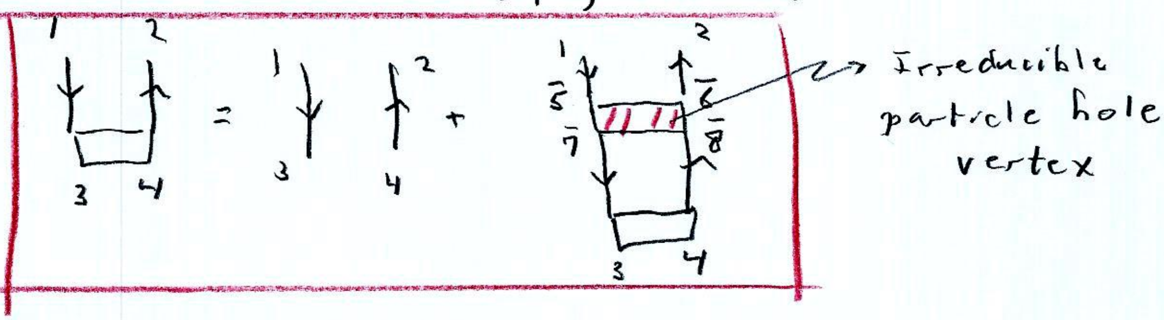
$$\frac{\delta \mathcal{G}}{\delta \varphi} = -\mathcal{G}\,\frac{\delta \mathcal{G}^{-1}}{\delta \varphi}\,\mathcal{G} \qquad \text{but } \mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \varphi - \Sigma$$

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

$$\frac{\delta \mathcal{G}(1,2)}{\delta \varphi(3,4)} = \mathcal{G}(1,\bar{2})\,\frac{\delta \varphi(\bar{2},\bar{3})}{\delta \varphi(3,4)}\,\mathcal{G}(\bar{3},2)$$




$$+\,\mathcal{G}(1,\bar{5})\,\frac{\delta \Sigma(\bar{5},\bar{6})}{\delta \mathcal{G}(\bar{7},\bar{8})}\,\frac{\delta \mathcal{G}(\bar{7},\bar{8})}{\delta \varphi(3,4)}\,\mathcal{G}(\bar{6},2)$$

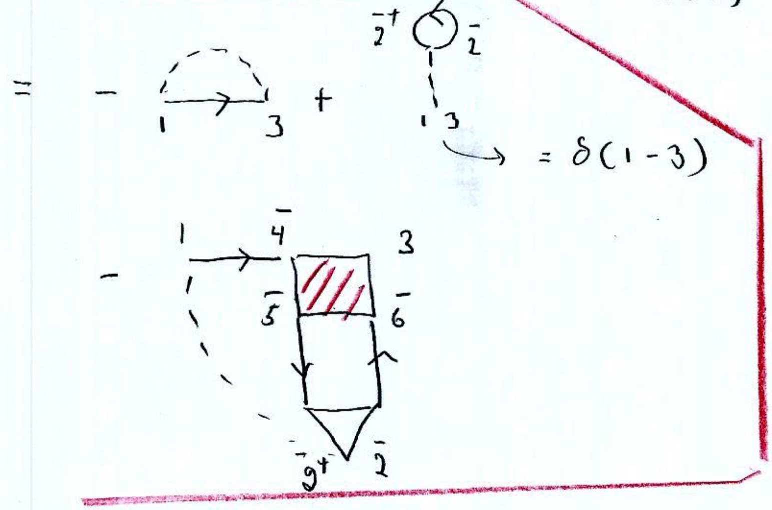


## 36.4 Self-energy from functional derivative

$$\Sigma(1,3) = -V(1-\bar{2})\left[\frac{\delta \mathcal{G}(1,\bar{3})}{\delta\phi(\bar{2}^+,\bar{2})} - \mathcal{G}(1,\bar{3})\,\mathcal{G}(\bar{2}^+,\bar{2})\right]\mathcal{G}^{-1}(\bar{3},3)$$

$$= -V(1-\bar{2})\left[\mathcal{G}(1,\bar{2}^+)\,\mathcal{G}(\bar{2},\bar{3}) + \mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\,\frac{\delta\mathcal{G}}{\delta\phi}\right)\mathcal{G} - \right.$$

$$\left. - \mathcal{G}(1,\bar{3})\,\mathcal{G}(\bar{2}^+,\bar{2})\right]\mathcal{G}^{-1}(\bar{3},3)$$



# GW + TPSC + others

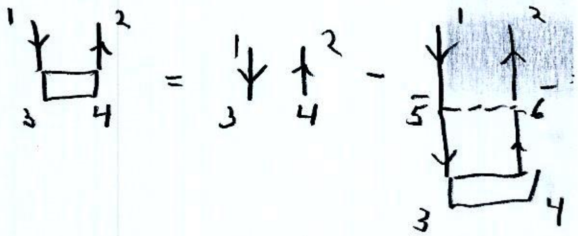
(90 minutes)

Summary

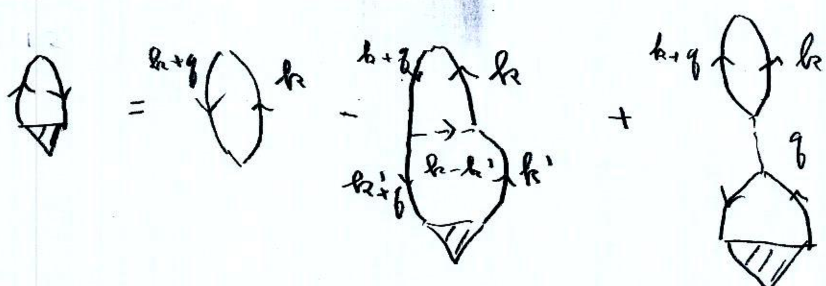
## Cours #6

## Chapter 37 Hartree-Fock + RPA Long-Range forces

### 37.2 Hartree-Fock + RPA in space-time




### 37.3 Hartree-Foch + RPA in momentum-Matsubara space

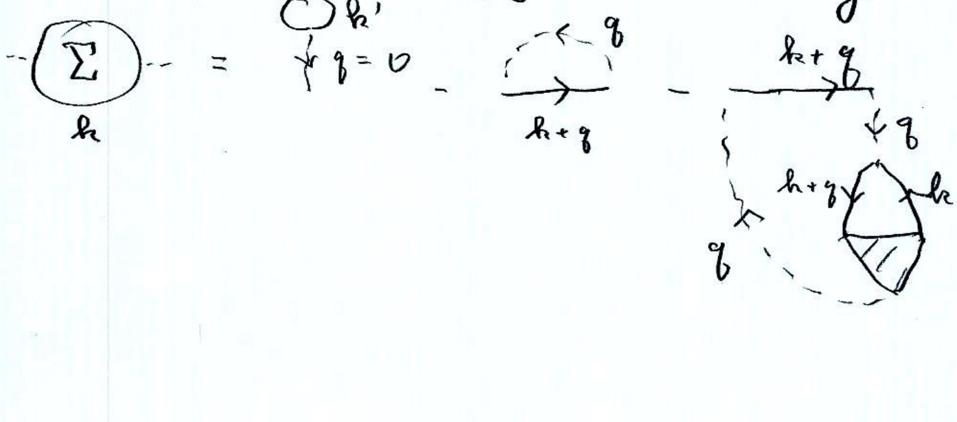



### 39.3 Density response in noninteracting limit

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

### 41.1.2 RPA

## 44. Second step Self-energy and screening and GW



# 56 Hubbard in the footsteps of the electron gas

Summary

## 56.2 Response functions

$$U_{sp} = \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\downarrow} - \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\uparrow} \quad ; \quad U_{ch} = \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\downarrow} + \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\uparrow}$$

## 56.3 Hartree-Fock and RPA

$$\chi_{sp} = \frac{\chi_0}{1-\frac{U}{2}\chi_0} \quad ; \quad \chi_{ch} = \frac{\chi_0}{1+\frac{U}{2}\chi_0}$$

## 56.4 RPA and violation of Pauli exclusion

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

## 56.6 RPA, phase transitions + Mermin-Wagner

$$q^2\langle S^z_q S^z_{-q}\rangle = \frac{T}{2} \qquad \langle S_z^2\rangle = \int_0^\infty \frac{d^2q}{q^2}\,\frac{T}{2} = \infty$$

# 57 Two-particle self-consistent TPSC

## 57.1 TPSC first step, spin + charge

$$U_{sp} = U\,\frac{\langle n_\uparrow n_\downarrow\rangle}{\langle n_\uparrow\rangle\langle n_\downarrow\rangle} \quad ; \quad U_{ch} \text{ from Pauli}$$

## 57.2 Improved self

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

## 57.3 Internal consistency check

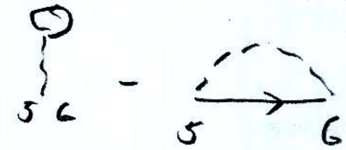
$$\Sigma_\sigma(1,\bar{1})\,\mathcal{G}_\sigma(\bar{1},1^+) = \frac{1}{2}\operatorname{Tr}(\Sigma\mathcal{G}) = U\langle n_\uparrow n_\downarrow\rangle$$

$$\frac{1}{2}\operatorname{Tr}\left[\Sigma^{(2)}\mathcal{G}^{(1)}\right] = U\langle n_\uparrow n_\downarrow\rangle$$

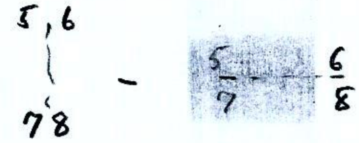
# 37. Long-range forces

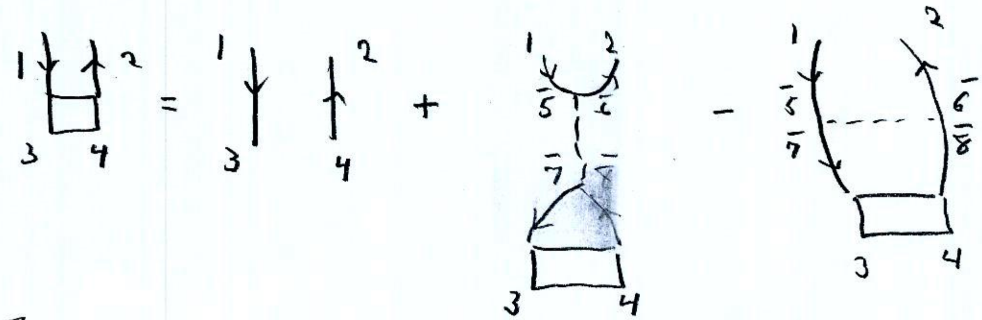
## 37.2 Hartree-Fock and RPA in space-time

$\Sigma(5,6) =$

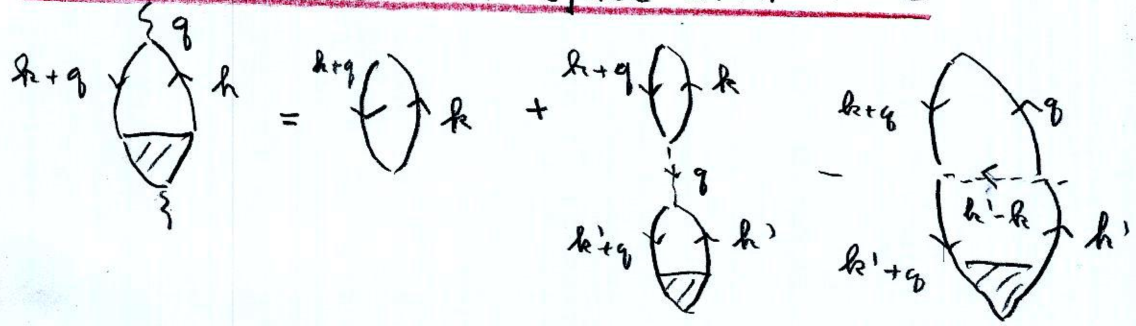


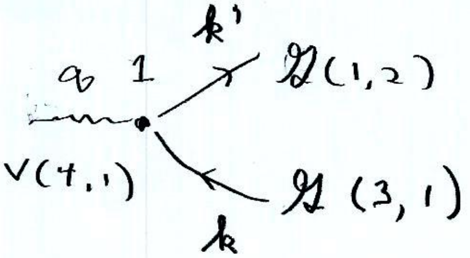

$$\frac{\delta \Sigma(5,6)}{\delta \mathcal{G}(7,8)} =$$




## 37.3 In momentum space with $\varphi = 0$




$$\int d1 \int dk' e^{ik'\cdot 1} \int dk\, e^{-ik\cdot 1} \int dq\, e^{-iq\cdot 1}$$

$$\Rightarrow \delta\left(k' - (k+q)\right)$$

Conservation of 4-momentum at every vertex

Sum over all frequency-wave vector not determined by conservation

## 39.3 Density response in non-interacting limit

Lindhard function.

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

$$= \sum_{\sigma_1\sigma_2} \langle T_\tau \psi^\dagger(1^+)\psi(1)\psi^\dagger(2^+)\psi(2)\rangle - n^2$$

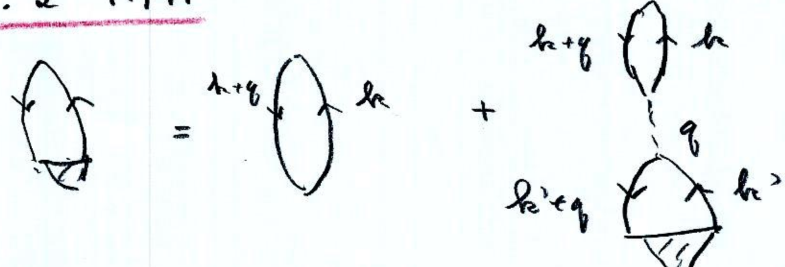
$\chi^0_{nn}(q) = -$  Also seen with Wick.

$$\chi^0_{nn}(q) = -2\frac{T}{N}\sum_{ik_n}\sum_{k}\left[\frac{1}{ik_n+iq_n-\zeta_{k+q}}\;\frac{1}{ik_n-\zeta_k}\right]$$

$$= -\frac{2T}{N}\sum_{k}\sum_{ik_n}\left[\frac{1}{ik_n+iq_n-\zeta_{k+q}} - \frac{1}{ik_n-\zeta_k}\right]\frac{1}{\zeta_{k+q}-\zeta_k-iq_n}$$

$$\boxed{= \frac{2}{N}\sum_{k}\frac{f(\zeta_{k+q})-f(\zeta_k)}{iq_n-(\zeta_k-\zeta_{k+q})}}$$

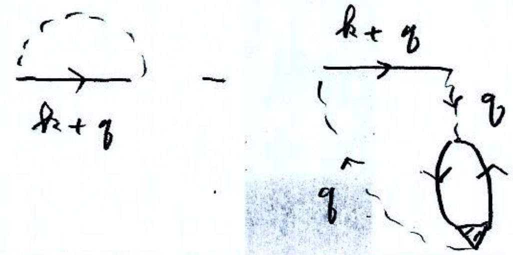
## 41.1.2 RPA



$$-\chi_{nn} = -\chi^0_{nn} + (-\chi^0_{nn})\,V(q)\,(-\chi_{nn})$$

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

## 44. Second step: GW, curing Hartree Fock

$\Sigma = -$ 


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

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

## 56. Hubbard model in the footsteps of the electron gas

### 56.2 Response functions

$$\frac{\delta \mathcal{G}_\sigma}{\delta \varphi_{\sigma'}} = \mathcal{G}_\sigma \mathcal{G}_\sigma \delta_{\sigma\sigma'} + \mathcal{G}_\sigma \left[ \frac{\delta \Sigma_\sigma}{\delta \mathcal{G}_{\bar\sigma}} \frac{\delta \mathcal{G}_{\bar\sigma}}{\delta \varphi_{\sigma'}} \right] \mathcal{G}_\sigma$$

$$\chi_{ch}(1,2) = -\sum_{\sigma\sigma'} \frac{\delta \mathcal{G}_\sigma(1,1^+)}{\delta \varphi_{\sigma'}(2^+,2)} \Rightarrow \chi^0 = -2\mathcal{G}\mathcal{G}$$

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

$$U_{sp}(1,2;3,4) = \frac{\delta \Sigma_\uparrow(1,2)}{\delta \mathcal{G}_\downarrow(3,4)} - \frac{\delta \Sigma_\uparrow(1,2)}{\delta \mathcal{G}_\uparrow(3,4)}$$

$$U_{ch} = \frac{\delta \Sigma_\uparrow}{\delta \mathcal{G}_\downarrow} + \frac{\delta \Sigma_\uparrow}{\delta \mathcal{G}_\uparrow}$$

$$\boxed{\chi_{\underset{sp}{ch}} = \chi^0_{\underset{sp}{ch}} \underset{+}{-} \chi^0_{\underset{sp}{ch}} U_{\underset{sp}{ch}} \chi_{\underset{sp}{ch}}}$$

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## 56.3 Hartree-Fock + RPA

$$\Sigma^{H}_{\sigma}(1,2)_{\varphi} = U\, \mathcal{G}^{H}_{-\sigma}(1,1^{+})_{\varphi}\, \delta(1-2)$$

$$\frac{\delta \Sigma^{H}_{\uparrow}}{\delta \mathcal{G}^{H}_{\uparrow}} = 0 \qquad \frac{\delta \Sigma^{H}_{\uparrow}}{\delta \mathcal{G}_{\downarrow}} = U$$

$$\chi_{\substack{sp \\ ch}} = \frac{\chi^{0}}{1 \mp \frac{U}{2}\chi^{0}} \qquad \chi^{0}(1,2) = -2\,\mathcal{G}^{H}(1,2)\,\mathcal{G}^{H}(2,1)$$

$$\chi^{0}(q) = -2\sum_{k} \mathcal{G}^{H}(k)\,\mathcal{G}^{H}(k+q)$$

## 56.4 RPA and violation of the Pauli principle

$$\frac{T}{N}\sum_{q,iq_n} \chi_{sp}(q,iq_n) = \langle (n_\uparrow - n_\downarrow)^2\rangle = \langle n\rangle - 2\langle n_\uparrow n_\downarrow\rangle$$

$$\frac{T}{N}\sum_{q,iq_n} \chi_{ch}(q,iq_n) = \langle (n_\uparrow + n_\downarrow)^2\rangle - \langle n\rangle^2 = \langle n\rangle + 2\langle n_\uparrow n_\downarrow\rangle - \langle n\rangle^2$$

$$\frac{T}{N}\sum_{q,iq_n}\left[\frac{\chi^{0}}{1-\frac{U}{2}\chi^{0}} + \frac{\chi^{0}}{1+\frac{U}{2}\chi^{0}}\right] \neq 2\langle n\rangle - \langle n\rangle^2$$

$$\mathcal{O}(U^2)$$

## 56.C RPA, phase transitions and Mermin-Wagner

$$1 = \frac{U}{2}\chi^{0} \Rightarrow \text{divergence} \Rightarrow \text{phase transition}$$

Hubbard model at half-filling $t' = 0$ $\quad \chi^{0} \propto N(0)\ln\left(\frac{E_F}{T}\right)$

divergence at finite $T$

Mermin-Wagner

$$q^2 \langle S_z(q) S_z(-q)\rangle \propto k_B T$$

$$\boxed{\langle S_z^2\rangle = \int d^2q\, \frac{k_B T}{q^2} = \infty}$$

# 57. Two-particle self-consistent TPSC

## 57.1 First step: spin and charge fluctuations

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

If $1 \neq 2$ $\quad \Sigma^{(1)}_\sigma \mathcal{G}^{(1)}_\sigma = A_\varphi \mathcal{G}^{(1)}_\sigma \mathcal{G}^{(1)}_\sigma$

If $2 = 1^+$ $\quad \Sigma^{(1)}_\sigma \mathcal{G}^{(1)}_\sigma = U \langle n_\uparrow n_\downarrow\rangle$

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

$$\Sigma^{(1)}_\sigma(1,2)_\varphi = \frac{U\langle n_\uparrow n_\downarrow\rangle_\varphi}{\langle n_\uparrow\rangle_\varphi\langle n_\downarrow\rangle_\varphi}\mathcal{G}^{(1)}(1,1^+)\,\delta(1-2)$$

$$\boxed{\frac{\delta\Sigma^{(1)}_\uparrow(1,2)_\varphi}{\delta\mathcal{G}_\downarrow(3,4)_\varphi} - \frac{\delta\Sigma^{(1)}_\uparrow(1,2)_\varphi}{\delta\mathcal{G}_\uparrow(3,4)_\varphi} = \frac{U\langle n_\uparrow n_\downarrow\rangle}{\langle n_\uparrow\rangle\langle n_\downarrow\rangle}\delta(1-2)\delta(3-1)\delta(4-2)}$$

$$\boxed{U_{sp} = \frac{U\langle n_\uparrow n_\downarrow\rangle}{\langle n_\uparrow\rangle\langle n_\downarrow\rangle}\ ; \quad U_{ch} \text{ determined by Pauli}}$$

## 57.2 An improved self-energy

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

Right-multiply by $\mathcal{G}^{-1}$ and use $\frac{\delta \mathcal{G}}{\delta\varphi}\mathcal{G}^{-1} = -\mathcal{G}\frac{\delta \mathcal{G}^{-1}}{\delta\varphi}$ $\Rightarrow$

$$\Sigma^{(2)}_\sigma(1,2) = U\mathcal{G}^{(1)}_{-\sigma}(1,1^+)\delta(1-2)$$
$$- U\mathcal{G}^{(1)}_\sigma(1,\bar{3})\left[\frac{\delta\Sigma^{(1)}_\sigma(\bar{3},2)}{\delta\mathcal{G}^{(1)}_{\bar{\sigma}}(\bar{4},\bar{5})}\frac{\delta\mathcal{G}^{(1)}_{\bar{\sigma}}(\bar{4},\bar{5})}{\delta\varphi_{-\sigma}(1^+,1)}\right]_{\varphi=0}$$

Do the same in transverse channel

Assume crossing symmetry

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

## 57.3 Internal accuracy check

$$\Sigma_\sigma(1,\bar{1})\mathcal{G}_\sigma(\bar{1},1^+) = \frac{1}{2}\mathrm{Tr}\left[\Sigma\mathcal{G}\right] = U\langle n_\uparrow n_\downarrow\rangle$$

Exact $\quad \frac{1}{2}\mathrm{Tr}\left[\Sigma^{(2)}\mathcal{G}^{(1)}\right] = U\langle n_\uparrow n_\downarrow\rangle$ exact

$\frac{1}{2}\mathrm{Tr}\left[\Sigma^{(2)}\mathcal{G}^{(2)}\right] \overset{?}{=} U\langle n_\uparrow n_\downarrow\rangle$ internal accuracy check

# Iterated perturbation theory

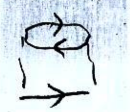
8 juin 2022 (44)

(Anderson impurity) H. Kajueter G. Kotliar PRL 77, 131 (96)

Green function that takes into account the bath

$$\mathcal{G}_0^{-1} = ik_n + \tilde{\mu} - \Delta(ik_n)$$

allows to compute $\Sigma$ to second-order in $U$

Call this $\Sigma^{(2)}(ik_n)$ 

Take for the self

$$\Sigma_{int} = U n_{-\sigma} + \frac{A\,\Sigma^{(2)}}{1 - B\,\Sigma^{(2)}}$$

Choose $A$ and $B$ to reproduce:

- Atomic limit
- Exact first 2 terms of high frequency expansion

High-frequency expansion

$$\mathcal{G}_k(ik_n) = \int \frac{d\omega}{2\pi} \frac{A_k(\omega)}{ik_n - \omega} \sim \frac{1}{ik_n}\int \frac{d\omega}{2\pi} A_k(\omega) + \frac{1}{(ik_n)^2}\int \frac{d\omega}{2\pi}\omega^2 A_k(\omega)$$

$$+ \frac{1}{(ik_n)^3}\int \frac{d\omega}{2\pi}\omega^2 A_k(\omega)$$

Moments from equal-time commutators

$$A_k(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} A_k(\omega) = \langle\{c_k(t), c_k^\dagger\}\rangle$$

$$i\frac{\partial A_k(t)}{\partial t} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t}\,\omega A_k(\omega) = i\langle\{\frac{\partial c_k(t)}{\partial t}, c_k^\dagger\}\rangle$$

$$i^2\frac{\partial^2 A(t)}{\partial t^2} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t}\,\omega^2 A_k(\omega) = i^2\langle\{\frac{\partial^2 c_k(t)}{\partial t^2}, c_k^\dagger\}\rangle$$

$$i \frac{\partial c_k(t)}{\partial t} = i \frac{\partial}{\partial t} \left[ e^{iHt} c_k e^{-iHt} \right]$$

$\Rightarrow$ evaluated from equal-time commutator.

Expanding $\frac{1}{ik_n + \mu - \epsilon_k - \Sigma(ik_n)} = \mathcal{G}_k(ik_n)$

$\Sigma = a + \frac{b}{ik_n}$ and equating with above

$$\Sigma = U n_{-\sigma} + U^2 \frac{n_{-\sigma}(1 - n_{-\sigma})}{ik_n}$$

Once A and B are chosen, $\tilde{\mu}_0$ still free to vary

- at $T=0$, enforce $n$ lattice $= n_0$

(Luttinger's theorem or Friedel sum rule)

- at $T \neq 0$ $n = n_0$ any way
- This has problems for electron doping at large U

Use instead

$$T \sum_n \Sigma_{int}(ik_n) \mathcal{G}_{int}(ik_n) = U \langle n_\uparrow n_\downarrow \rangle$$

L.F. Arsenault PRB 86, 085133 (2012)

$U\langle n_\uparrow n_\downarrow \rangle$ from exact result
or from large U limit.