Lectures: Why

#1. Second quantization (45 min)

- Useful if more than 1. Slater determinant

#2. Green's functions (45 min)

- Necessary for perturbation theory
- Connected to photoemission.
- Hubbard model

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

- GW (Brunival, Kotliar)
- Many-body perturbation theory

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

- Derivation DMFT (Sénéchal)
- Proofs CTQMC (Ferrero)

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

- GW
- Luttinger Ward
- TPSC (Hubbard, weak to intermediate)

#1

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Ecole d'été 2018

67. Second quantization

67.1 Creation-annihilation operators

Number operator

67.2 Change of basis

Position and momentum basis

Wave functions

67.3 One-body operators

67.4 Two-body operators

Important results:

- Why second quatization

Apply $L \to p = \frac{\partial L}{\partial \dot{q}}$ $[q, p] = i\hbar$ → N.B. "Scales" i.e. center of mass as well

to Ψ Schrödinger, like apply to $\vec{E}$ field

- Here pedestrian approach ⇒ wave-particle duality

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

$$[n_\alpha, a^+_\alpha] = a^+_\alpha \qquad [\hat{n}_\alpha, a_\alpha] = -a_\alpha$$

- Change of basis

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

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

- $\Psi^+(r)|0\rangle = |r\rangle \Rightarrow$

$$\langle 0 | \Psi(r') \Psi^+(r) | 0 \rangle = \langle r' | r \rangle = \delta(r - r')$$

- Wave function

$$\langle r_1 \cdots r_N | \alpha_1 \cdots \alpha_N \rangle = \det \begin{bmatrix} \varphi_{\alpha_1}(r_1) & \varphi_{\alpha_1}(r_2) & \cdots & \varphi_{\alpha_1}(r_N) \\ \vdots & & & \\ \varphi_{\alpha_N}(r_1) & \cdots & & \varphi_{\alpha_N}(r_N) \end{bmatrix}$$

- One body:

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

$$\hat{T} = \int d^3r \left(-\frac{\hbar^2}{2m}\right) \Psi^+(r) \nabla^2 \Psi(r)$$

- Two-body $V = \frac{1}{2} \sum_{\sigma\sigma'} \int d^3x \, d^3y \, v(x-y) \Psi^+_\sigma(x) \Psi^+_{\sigma'}(y) \Psi_{\sigma'}(y) \Psi_\sigma(x)$

67 Second quatization

67.1 Creation-annihilation operators

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

2 particles:

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

Creation operator:

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

$a^+_{\alpha_1}$ adds particle in state α_1 and antisymmetrizes

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

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

- Initial order arbitrary
- Work if interchange any two in the list

Annihilation :

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

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

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

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

Number operator

$$\hat{n}_\alpha \equiv a^+_\alpha a_\alpha$$

$$\boxed{\begin{array}{c} n_\alpha a^+_\beta = a^+_\beta n_\alpha \\ \text{thanks to (1), (2)} \end{array}}$$

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

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

$$= a^+_\alpha (1 - a^+_\alpha a_\alpha) | 0 \rangle$$

$$= a^+_\alpha | 0 \rangle$$

Works for any state $a^+_{\alpha_1} a^+_{\alpha_2} \cdots a^+_\alpha \cdots a^+_{\alpha_N} | 0 \rangle$

$$[\hat{n}_\alpha , a^+_\alpha] = a^+_\alpha \qquad [\hat{n}_\alpha , a_\alpha] = - a_\alpha$$

67.2 Change of basis

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

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

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

67.2.1 Position, momentum basis

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

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

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

67.2.2 Wave function

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

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

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

Example of non-zero term

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

and all possible permutations

thus $\Psi_{\alpha_1\cdots\alpha_N}(r_1\cdots r_N) =$

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

67.3 One-body operators

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

Example: (first quantized) in diagonal basis.

$$V(R_1) + V(R_2) + V(R_3)\,|r\,r'\,r''\rangle$$

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

In general in diagonal basis

$$\sum_m U_{\alpha_m}\hat{n}_{\alpha_m} = \sum_m \langle\alpha_m|\hat{U}|\alpha_m\rangle\,\hat{n}_{\alpha_m}$$

$$= \sum_m c^+_{\alpha_m}\langle\alpha_m|\hat{U}|\alpha_m\rangle\, c_{\alpha_m}$$

Change basis $= \sum_{ij} c^+_i \langle i|\hat{U}|j\rangle\, c_j$

Potential energy

$$\boxed{\begin{aligned}\hat{V} &= \int d^3r\; V(r)\,\psi^+(r)\,\psi(r)\\ \hat{T} &= \int d^3r\,\left(-\frac{\hbar^2}{2m}\right)\psi^+(r)\,\nabla^2\psi(r)\end{aligned}}$$

67.4 Two-body (Coulomb)

Diagonal basis

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

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

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

$$\boxed{\hat{V}_{\text{Coulomb}} = \frac{1}{2}\sum_{\sigma\sigma'}\int d^3x\,d^3y\; v(x-y)\,\psi^+_\sigma(x)\,\psi^+_{\sigma'}(y)\,\psi_{\sigma'}(y)\,\psi_\sigma(x)}$$

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

69. Perturbation theory $\boxed{e^{-\beta \hat{K}} = e^{-\beta K_0} T_\tau \left[e^{-\int_0^\beta d\tau \hat{K}_1(\tau)} \right]}$

70. Green functions

70.1 Photoemission $\boxed{\frac{\partial^2 \sigma}{\partial \Omega \, d\omega} \propto \int dt \, e^{-i\omega t} \langle c^{+}_{k}(t) c_{k} \rangle}$

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

70.3 Matsubara frequency $\boxed{\int_0^\beta d\tau \, e^{ik_n \tau} \mathcal{G}_{\alpha\beta}(\tau)}$

70.5 $\mathcal{G}$ for $U = 0$ $\boxed{\mathcal{G}(ik_n) = (ik_n - \xi_k)^{-1}}$

68.1. Hubbard model

For a solid: $\psi^{+}_{\sigma}(\vec{r}) = \sum_{n} \sum_{R_i} c^{+}_{i\sigma} \, w^{*}_{n}(\vec{r} - \vec{R}_i)$

Wannier state

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

Keep one band only

$$\hat{T} = \int d^3r \left(-\frac{\hbar^2}{2m} \right) \sum_{R_i} \sum_{R_j} c^{+}_{i\sigma} \, w_n(r - R_i) \nabla^2 w(r - R_j) \, c_{j\sigma}$$

$$= \sum_{R_i R_j} c^{+}_{i\sigma} \langle i | \frac{P^2}{2m} | j \rangle c_{j\sigma} = \sum_{ij} t_{ij} c^{+}_{i\sigma} c_{j\sigma}$$

Similarly

$$\hat{V} = \frac{1}{2} \sum_{\sigma\sigma'} \sum_{ijkl} \langle i | \langle j | v(\hat{x} - \hat{y}) | k \rangle | l \rangle \; c^{+}_{i\sigma} c^{+}_{j\sigma'} c_{l\sigma'} c_{k\sigma}$$

Same site only:

$$\hat{V} = \frac{1}{2}\sum_{\sigma\sigma'}\sum_i U\, c^+_{i\sigma}\, c^+_{i\sigma'}\, c_{i\sigma'}\, c_{i\sigma} = \sum_i U\, n_{i\uparrow} n_{i\downarrow}$$

Ground state:

$t=0$ $\quad |\Psi\rangle_{t=0} = \prod_{i\sigma_i} c^+_{i\sigma_i} |0\rangle$ Highly degenerate

$U=0$ $\quad |\Psi\rangle_{U=0} = \prod_k c^+_{k\uparrow}\, c^+_{k\downarrow} |0\rangle$

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

69. Perturbation theory and time-ordered product

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

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

$$\boxed{\begin{aligned} e^{-\beta\hat{K}} &= e^{-\beta\hat{K}_0}\,\hat{U}(\beta) \\ \hat{U}(\beta) &= T_\tau\left[e^{-\int_0^\beta d\tau\,\hat{K}_1(\tau)}\right] \\ K_1(\tau) &= e^{K_0\tau}\,K_1\,e^{-K_0\tau} \end{aligned}}$$

Proof:

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

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

$$\frac{\partial\hat{U}(\tau)}{\partial\tau} = -K_1(\tau)\,\hat{U}(\tau)$$

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

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

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

Recover exponential by defining T_τ time ordering operator and allowing $n!$ possible orders

70. Green functions contain useful information

Results of experiment related to correlation functions

70.1 Photoemission and fermion correlation function

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

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

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

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

$$\vec{j}_{q=0} \propto \sum_p \frac{\vec{p}}{m} c^+_p c_p \qquad \text{drop spin}$$

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

$$\propto \int dt \, e^{-i\omega t} \sum_{mn} \frac{e^{-\beta K_m}}{Z} \langle m| e^{iKt/\hbar} c^+_{k_{\parallel}} e^{-iKt/\hbar} |n\rangle \langle n| c_{k_{\parallel}} |m\rangle$$

$$\propto \int dt \, e^{-i\omega t} \, \mathrm{Tr}\left[\rho \, c^+_{k_{\parallel}}(t) \, c_{k_{\parallel}}\right]$$

$$\equiv \int dt \, e^{-i\omega t} \langle c^+_{k_{\parallel}}(t) \, c_{k_{\parallel}} \rangle$$

70.2 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_τ motivated by perturbation theory

$$\langle \mathcal{O}\rangle = T_r[\rho\,\mathcal{O}]$$

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

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

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

70.3 Matsubara frequency representation is convenient

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

Proof: Let $\tau > 0$, then

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

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

Using the theorem on Fourier series

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

10.5 $\mathcal{G}(ik_n)$ for $U=0$

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

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

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

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

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

$$= -\xi_k c_k(\tau)$$

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

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

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

$$\text{Since } -\mathcal{G}_k(0^+) = \langle c_k c_k^+\rangle$$

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

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

$$\text{and } \langle c_k c_k^+\rangle + \langle c_k^+ c_k\rangle = 1$$

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

$\boxed{\#3}$

70.4 Spectral weight, relation to photoemission $\boxed{\frac{\partial^2\sigma}{\partial\Omega\partial\omega} \propto A_k(\omega) f(\omega)}$

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

71. Self-energy and the effect of interactions

71.1 The atomic limit $\boxed{\frac{1-\langle n\rangle}{ik_n+\mu} + \frac{\langle n\rangle}{ik_n+\mu-U}}$

71.2 Self-energy and atomic limit

Dyson's equation $\boxed{[G^R]^{-1} = [G^0]^{-1} - \Sigma^R}$

71.3 A few properties $\boxed{\mathrm{Im}\,\Sigma^R < 0}$

71.4 Anderson impurity problem

$\boxed{[G^R]^{-1} = [G^0]^{-1} - \Delta - \Sigma^R}$

70.4 Spectral weight and relation to photoemission

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

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

Lehmann

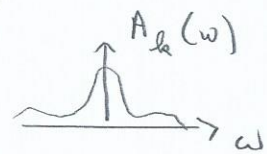
$$\boxed{\mathcal{G}(ik_n) = \int \frac{d\omega}{2\pi} \frac{A_k(\omega)}{ik_n - \omega}}$$

$A_k(\omega)$ = spectral weight

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

Spectral weight is normalized:

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



For free particle:

$K_n - K_m = \xi_k$ only allowed case $\Rightarrow$

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

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

Photoemission:

Photoemission:

We also have

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

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

70.6 $A_k(\omega)$ from $\mathcal{G}$: analytical continuation

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

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

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

7I. Self-energy and the effect of interactions

7I.1 The atomic limit $t=0$

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

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

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

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

Spectral weight from top formula on p. 13:

$$\hat{K}|0\rangle = 0 \qquad \hat{K}|\uparrow\downarrow\rangle = (U-2\mu)|\uparrow\downarrow\rangle$$

$$\hat{K}|\sigma\rangle = -\mu|\sigma\rangle$$

Only $|m\rangle = |\uparrow\rangle$ and $|\uparrow\downarrow\rangle$ contribute to $c_\uparrow|m\rangle$

Also $\frac{1}{N}\sum_{r_i r_j} e^{ik\cdot(r_i - r_j)} G_\sigma(r_i - r_j) = G_{k\sigma} = G_\sigma(0)$

So
$$A_{k\uparrow}(\omega) = \frac{e^{\beta\mu}}{Z}(1+e^{\beta\omega})\, 2\pi\, \delta(\omega - (-\mu)) \quad \left\{ \begin{array}{l} |m\rangle = |\uparrow\rangle \\ |n\rangle = |0\rangle \end{array} \right.$$

$$+ \frac{e^{\beta(2\mu-U)}}{Z}(1+e^{\beta\omega})\, 2\pi\, \delta(\omega - ((U-2\mu)+\mu))$$

$$\left\{ \begin{array}{l} |m\rangle = |\uparrow\downarrow\rangle \\ |n\rangle = |\downarrow\rangle \end{array} \right.$$

$$= \frac{(1+e^{\beta\mu})}{Z}\, 2\pi\, \delta(\omega+\mu)$$

$$+ \frac{e^{\beta(2\mu-U)} + e^{\beta\mu}}{Z}\, 2\pi\, \delta(\omega+\mu-U)$$

$$\boxed{= (1-\langle n_\uparrow\rangle)\, 2\pi\, \delta(\omega+\mu) + \langle n_\uparrow\rangle\, 2\pi\, \delta(\omega+\mu-U)}$$

Alternatively

71. Self-energy and the effect of interactions

71.1 The atomic limit, $t=0$

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

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

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

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

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

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

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

$$\boxed{\int_0^\beta d\tau\, e^{ik_n\tau} G_{k\uparrow}(\tau) = G_{k\uparrow}(i\omega_n)}$$

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

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

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

7.2 Self-energy

For the general case, we define the self-energy by:

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

Effect of interactions

Why? Because it has a natural interpretation as a lifetime caused by interactions

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

Dyson's equation:

In the non-interacting case:

$$\left[G^{R0}_{k\sigma}(\omega)\right]^{-1} = \omega + i\eta - \xi_{k\sigma}$$

Hence:

$$\left(\left[G^{R0}_{k\sigma}(\omega)\right]^{-1} - \Sigma^R_{k\sigma}(\omega)\right) G^R_{k\sigma}(\omega) = 1$$

or:

$$G^R_{k\sigma}(\omega) = G^{R0}_{k\sigma}(\omega) + G^{R0}_{k\sigma}(\omega)\,\Sigma_{k\sigma}(\omega)\,G^R_{k\sigma}(\omega)$$

7.3 A few properties:

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

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

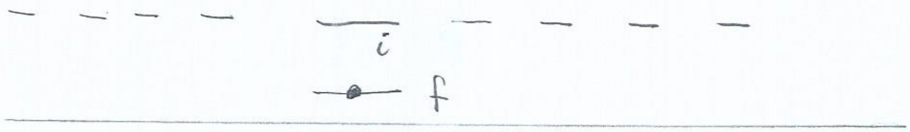
13.4 "Integrating out the bath": Anderson impurity

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

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

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

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



Note:

$$[U f^+_{i\downarrow} f_{i\downarrow} f^+_{i\uparrow} f_{i\uparrow}, f_{i\uparrow}] = - U f^+_{i\downarrow} f_{i\downarrow} f_{i\uparrow}$$

since $[n_{i\downarrow}, f_{i\downarrow}] = - f_{i\downarrow}$

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

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

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

In Matsubara frequency, use equation for $\mathcal{G}_{cf\sigma}$ in terms of $\mathcal{G}_{ff}$ in the equation for $\mathcal{G}_{ff}$ to have an equation only in terms of $\mathcal{G}_{ff}$:

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

Hybridation function: $\boxed{\Delta(ik) \equiv \sum_k V^*_{ik} \frac{1}{ik_n - (\epsilon_k - \mu)} V_{ki}}$

It is as if we had a time-dependent non-interacting Hamiltonian.
The action formalism is more suited.

Note: Interpretation in terms of summing over all trajectories

Note the matrix structure below:

$$
\begin{bmatrix}
ik_n-(\epsilon-\mu)-\Sigma_{ff\sigma}(ik_n) & -V^*_{ik_0} & -V^*_{ik_1} & \cdots \\
-V_{k_0 i} & ik_n-(\epsilon_{k_0}-\mu) & 0 & \cdots \\
-V_{k_1 i} & 0 & ik_n-(\epsilon_{k_1}-\mu) & \cdots \\
\vdots & & &
\end{bmatrix}
\begin{bmatrix}
G_{ff}(ik_n) \\
G_{cf\sigma}(k_0, i; ik_n) \\
G_{cf\sigma}(k_1, i; ik_n) \\
\vdots
\end{bmatrix}
=
\begin{bmatrix}
1 \\ 0 \\ 0 \\ \vdots
\end{bmatrix}
$$

#4 65. Coherent states for fermions. (see also 78)

65.1 Grassmann variables for fermions.

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

65.2 Grassmann integrals

$$\boxed{\int d\eta = 0 \;;\quad \int d\eta\,\eta = 1}$$

65.3 Change of variables in Grassmann integrals

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

65.4 Grassmann Gaussian integrals

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

$$\det[A] = \exp[\mathrm{Tr}\ln A]$$

65.5 Closure, overcompleteness, trace formula

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

66. Coherent state functional integral for fermions

66.1 Simple example single fermion

$$\boxed{Z = \int \mathcal{D}\eta^{+}\mathcal{D}\eta\; e^{-\int_0^\beta d\tau\left(\eta^{+}(\tau)\frac{\partial}{\partial\tau}\eta(\tau) + H(\eta^{+},\eta)\right)}}$$

66.3 Wick's theorem

$$(-1)^m\langle T_\tau c(\tau_m)c^{+}(\tau_m') \cdots c(\tau_2)c^{+}(\tau_2')c(\tau_1)c^{+}(\tau_1')\rangle$$
$$= \det\begin{bmatrix} \mathcal{G}(\tau_1,\tau_1')\,\mathcal{G}(\tau_1,\tau_2') \cdots \mathcal{G}(\tau_1,\tau_m') \\ \vdots \\ \mathcal{G}(\tau_m,\tau_1')\,\mathcal{G}(\tau_m,\tau_2') \cdots \mathcal{G}(\tau_m,\tau_m') \end{bmatrix}$$

66.5 Interactions and quantum impurities

$$\boxed{\mathcal{G}_{I}^{0\,-1} = ik_n - (\epsilon_i - \mu) - \sum_k V_{ik}^{*}\frac{1}{ik_n - (\epsilon_k - \mu)}V_{ki}}$$

65. Coherent states for fermions

65.1 Grassmann variables for fermions

$c|\eta\rangle = \eta|\eta\rangle$ by analogy with bosons, eigenstate of the destuction operator $c|0\rangle = 0$

Eigenvalues must be numbers that anticommute

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

$\{\eta_1, \eta_1^+\} = 0$ (since inside T_0)

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

$$c|\eta\rangle = c|0\rangle + \eta c c^+|0\rangle \quad \text{if } \{\eta, c\} = 0$$

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

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

65.2 Grassman integrals

All functions are at most first order in η

$$\int d\eta = 0 \quad \Rightarrow \quad \int d\eta\, f(\eta + \xi) = \int d\eta\, f(\eta) \quad \left(\text{also: } \int d\eta \frac{\partial f}{\partial \eta} = 0\right)$$

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

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

(product of 2 Grassmann numbers is an ordinary number)

65.3 Change of variables

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

$$\int d\psi_1\, d\psi_2 \ldots d\psi_N = \sum_{j_1=1}^{N} \cdots \sum_{j_N=1}^{N} U_{1j_1} U_{2j_2} \cdots U_{Nj_N} \int d\eta_{j_1} \cdots \int d\eta_{j_N}$$

$$= \sum_{j_1=1}^{N} \cdots \sum_{j_N=1}^{N} U_{1j_1} U_{2j_2} \cdots U_{Nj_N}\, \epsilon^{j_1 j_2 \cdots j_N} \int d\eta_1 \cdots \int d\eta_N$$

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

65.4 Grassman Gaussian integrals

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

$$= \exp(\ln a)$$

$$\int d\eta_1^+ \int d\eta_1 \int d\eta_2^+ \int d\eta_2\; \exp(-\eta_1^+ a_1 \eta_1 - \eta_2^+ a_2 \eta_2)$$

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

$$\boxed{\underbrace{\int \mathcal{D}\eta^+ \int \mathcal{D}\eta}_{\text{short-cut}}\; e^{-\eta^+ A \eta} = \det[A] = \exp[\mathrm{Tr} \ln A]}$$

Source field: (J is a Grassman variable)

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

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

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

65.5 Closure, overcompleteness, trace formula

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

$$= \int d\eta^+ \int d\eta \; \overbrace{(1-\eta^+\eta)\,(1-\eta c^+)\,\underbrace{|0\rangle\langle 0|}_{1}\,(1-c\eta^+)}^{2}$$

$$= \underbrace{|0\rangle\langle 0|}_{1} + |1\rangle\langle 1| \quad 2$$

65.5 Closure, overcompleteness, trace formula

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

$$= \int d\eta^+ \int d\eta \, e^{-\eta^+\eta} \langle 0 | (1 + c\eta^+) \, O \, (1 - \eta c^+) | 0 \rangle$$

$$= \int d\eta^+ \int d\eta \, (1 - \eta^+\eta) \left(\langle 0 | O | 0 \rangle - \eta^+\eta \langle 1 | O | 1 \rangle \right)$$

$$= \langle 0 | O | 0 \rangle + \langle 1 | O | 1 \rangle \qquad \left(\begin{array}{l} O \text{ has even \#} \\ \text{of fermions} \end{array} \right)$$

66 Coherent state functional integral for fermions

66.1 Simple example with single fermion.

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

Use trace formula and closure

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

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

where

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

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

Change of sign because of imaginary time

Start from the final result in the diagonal basis, then it is easy to see

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

Hence, in Matsubara basis:

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

66.3 Wick's theorem

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

$$= \mathcal{G}_{11}\mathcal{G}_{22}\cdots\mathcal{G}_{mm} \quad \text{in the diagonal basis.}$$

This is the determinant of the matrix. Hence, in an arbitrary basis,

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

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

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

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

66.5 Effective action for quantum impurity

$f \to \psi$
$c \to \eta$

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

$$S_I = \int_0^\beta d\tau \left[\sum_\sigma \left(\psi_\sigma^+(\tau) \frac{\partial}{\partial\tau} \psi_\sigma(\tau) + (\epsilon - \mu)\, \psi_\sigma^+(\tau) \psi_\sigma(\tau) \right] + U \psi_\uparrow^+(\tau) \psi_\downarrow^+(\tau) \psi_\downarrow(\tau) \psi_\uparrow(\tau) \right]$$

$$S_b = \int_0^\beta d\tau \sum_k \sum_\sigma \eta_\sigma^+(\vec{k},\tau) \left(-\mathcal{G}_b^{-1}(\vec{k},\tau) \right) \eta_\sigma(k,\tau)$$

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

We can make the correspondance with J on p. 21

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

Since the bath is quadratic, we can integrate over it. Then

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

Drops out from observables. See remark in the notes for subtleties.

In the diagonal basis,

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

$$= -\sum_n \sum_\sigma \psi_\sigma^+(ik_n)\, \Delta_\sigma(ik_n)\, \psi_\sigma(ik_n)$$

Hence

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

Hybridization expansion

Take two Matsubara frequencies (diagonal basis) to illustrate:

$$Z = C \int d\psi_1^+ \int d\psi_1 \int d\psi_2^+ \int d\psi_2 \; e^{-S_I} \underbrace{\left[(1 - \psi_1^+ \Delta_1 \psi_1)(1 - \psi_2^+ \Delta_2 \psi_2) \right]}_{\mathcal{U}}$$

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

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

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

In higher order terms, when we do the change of variables a given $\psi(\tau)$ or $\psi^+(\tau)$ must occur only once in a product.
But in going to imaginary time a given $\psi(\tau_i)$ may come from ψ_1 or from ψ_2. Similarly for $\psi^+(\tau_i)$. Reordering to get a fixed time order and taking care of anti-commutation will yield the determinant of Δ
Finally evaluating the final expression in the canonical formalism,

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

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

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

#5 Many-Body Perturbation Theory

Iterated perturbation theory

73. Source fields for many-body Green's function

73.1 A simple example from classical statistical mechanics (32.1)

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

73.2 Green's functions and higher order correlation functions

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

(32.2)

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

74.1 Equation of motion for $\psi(1)$ (33.1)

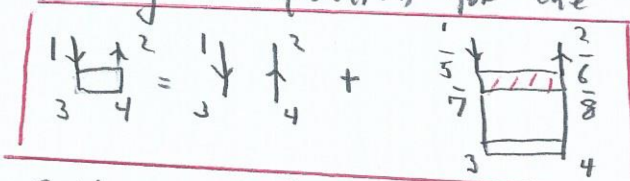
$$\boxed{\frac{\partial\psi(1)}{\partial\tau} = \frac{\nabla_1^2}{2m}\psi(1) + \mu\,\psi(1) - \psi^+(\bar{2})\,\psi(\bar{2})\,V(\bar{2}-1)\,\psi(1)}$$

74.2 Equation of motion for $\mathcal{G}_\varphi$ and def. of Σ_φ (33.2)

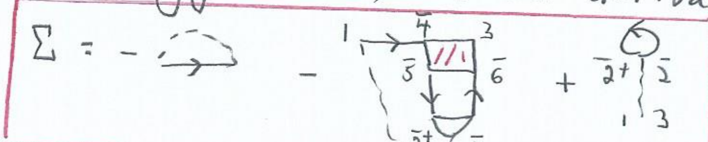
(*) See L.W. $$\boxed{\left[\mathcal{G}_0^{-1}(1,\bar{2}) - \varphi(1,\bar{2}) - \Sigma(1,\bar{2})_\varphi\right]\mathcal{G}(\bar{2},2)_\varphi = \delta(1-2)}$$

75. The general many-body problem

75.1 An integral equation for the 4-point function (33.3)

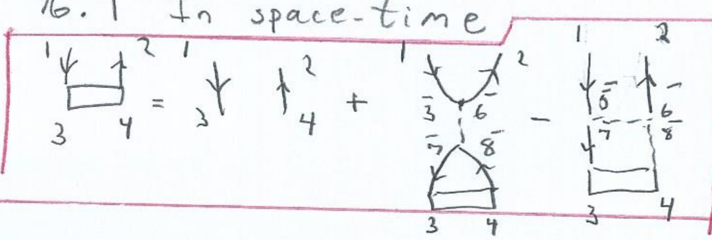


75.2 Self-energy from functional derivative (33.4)

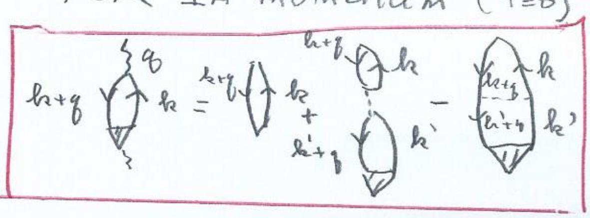


76. Long-range forces and GW (41.2)

76.1 In space-time

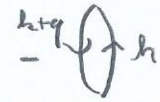


76.2 In momentum ($\varphi=0$)



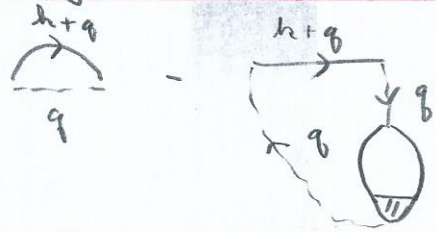
76.3 Density response in RPA (38.1.2)

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



76.4 Σ and screening in the GW approximation (41.2)

$$\Sigma = -$$



$$; \quad V_q \to \frac{V_q}{\frac{\epsilon(q, iq_n)}{\epsilon_0}}$$

61. Luttinger Ward and related functionals.

$$\boxed{\Omega[\mathcal{G}] = F[\varphi] - \mathrm{Tr}\,[\mathcal{G}\varphi] \quad ; \quad \frac{1}{T}\frac{\delta\Omega}{\delta\mathcal{G}(1,2)} = 0 \ \text{in equilibrium}}$$

62. Constraining-field method

62.1 Baym-Kadanoff-functional

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

$$\frac{\delta\Phi}{\delta\mathcal{G}} = \Sigma[\mathcal{G}] \quad ; \quad \Phi[\mathcal{G}] = \int_0^{e^2} de'^2\, \frac{1}{e'^2}\langle\hat{V}\rangle_{e'^2}$$

49. Hubbard model in the footsteps of the Electron gas

49.2 Response functions

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

49.3 Hartree-Fock and RPA

$$\boxed{\chi_{\substack{ch\\sp}} = \frac{\chi^0}{1 \mp \frac{U}{2}\chi^0} \qquad \chi^0(q) = 2\sum_k \mathcal{G}(k)\,\mathcal{G}(k+q)}$$

49.4 RPA and violation of Pauli

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

49.6 RPA and Mermin-Wagner

$$\boxed{q^2 \langle S_z(q) S_z(-q) \rangle = k_B T \quad \Rightarrow \quad \int d^2q \, \frac{k_B T}{q^2} = \langle S_z^2 \rangle = \infty}$$

50. Two-particle self-consistent approach

50.1 First step spin and charge fluctuations

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

50.2 An improved self-energy

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

50.3 TPSC Internal accuracy check

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

$$\stackrel{?}{=} \frac{1}{2} \mathrm{Tr} \left[\Sigma^{(2)} \mathcal{G}^{(2)} \right]$$

Iterated perturbation theory (Anderson impurity)

H. Kajueter and G. Kotliar, PRL 77, 131 (1996)

 → Green function that takes into account the bath

$$G_0^{-1} = ik_n + \tilde{\mu}_0 - \Delta(ik_n)$$

Allows to compute the self-energy to second-order in U

Call this $\Sigma_0^{(2)}(ik_n)$ (Later for perturbation theory)

 $= \Sigma^{(2)}$

$\mathcal{G}_\uparrow(\tau)\mathcal{G}_\downarrow(\tau)\mathcal{G}_\downarrow(-\tau)$

Take for the self-energy:

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

with A and B chosen to reproduce

- The atomic limit (seen previously)
- The exact first two terms of the high-frequency expansion

High frequency expansion

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

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

from the expression on p. 13 for $A_k(\omega)$, we find:

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

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

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

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

Hence it can be evaluated from equal-time commutators.

The moments can be obtained from $t=0$, i.e. equal-time anticommutators.

Expanding $$\frac{1}{ik_n+\mu-\epsilon_k-\Sigma_i(ik_n)} = G_k(ik_n)$$

with $\Sigma = a + \frac{b}{ik_n} + \ldots$ and equating with above, we find

$$\boxed{\Sigma_{int} = U n_{-\sigma} + U^2\frac{n_{-\sigma}(1-n_{-\sigma})}{ik_n} + \ldots}$$

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

- at $T=0$, enforce n for the lattice $= n_0$ (Luttinger theorem or Friedel sum rule)
- at $T\neq 0$, $n = n_0$
- This has problems for electron doping at large U. We can use instead (see later in these notes)

$$T\sum_n \Sigma_{int}(ik_n)\, G_{int}(ik_n) = U\langle n_\uparrow n_\downarrow\rangle$$

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

73. Source field to calculate many-body Green functions

73.1 A simple example from classical statistical mechanics

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

with operators that commute.

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

$$\frac{\delta h(x)}{\delta h(x')} = \delta(x-x')$$ 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, this is a way to compute correlation functions at $h=0$

73.2 Green functions and higher order correlation functions

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

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

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

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

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

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

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

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

74.1 Equations of motion for $\psi(1)$:

$$\frac{\partial \psi(1)}{\partial \tau} = \frac{\nabla_1^2}{2m}\psi(1) + \mu\psi(1) - \psi^+(\bar{2})\psi(\bar{2})V(\bar{2}-1)\psi(1)$$

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

74.2 Equation of motion for $\mathcal{G}_\varphi$ and def. of Σ_φ

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

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

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

61. Luttinger Ward and related functionals

$$F[\varphi] = -T \ln Z[\varphi] \quad \text{free energy}$$

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

Prefer to work in terms of observable $\mathcal{G}$ $\Rightarrow$ Legendre transform (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) $$\frac{1}{T}\frac{\delta \Omega}{\delta \mathcal{G}(1,2)} = -\varphi(2,1)$$

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

From equations of motion:

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

We thus have an extremum principle.

In equilibrium, $\varphi = 0$ and Dyson is satisfied

62. Constraining field method

62.1 Baym Kadanoff

General property of Legendre:

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

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

Here: $\left.\dfrac{\partial \Omega_{e^2}[\mathcal{G}]}{\partial \mathcal{G}}\right|_{\mathcal{G}} = \left.\dfrac{\partial F_{e^2}[\varphi]}{\partial e^2}\right|_{\varphi} = \underbrace{\dfrac{1}{e^2}\langle \hat{V} \rangle_{e^2}}_{\text{electron-electron interaction}}$

Hence

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

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

Where:

- Constraining field φ_0 is such that

  $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \varphi_0$ i.e. $\mathcal{G}$ is actual solution

- Luttinger-Ward functional

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

$$\boxed{\Omega_{e^2}[\mathcal{G}] = \underbrace{\mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_\infty}\right)\right]}_{F_{e^2=0}[\varphi_0]} - \mathrm{Tr}\left[\underbrace{(\mathcal{G}_0^{-1} - \mathcal{G}^{-1})}_{\varphi_0}\mathcal{G}\right] + \Phi_{e^2}[\mathcal{G}]}$$

$$\frac{\delta \Omega_{e^2}}{\delta \mathcal{G}} = 0 = \mathcal{G}^{-1} - \mathcal{G}_0^{-1} + \frac{\delta \Phi_{e^2}[\mathcal{G}]}{\delta \mathcal{G}} \Rightarrow \Sigma[\mathcal{G}] = \frac{\delta \Phi_{e^2}[\mathcal{G}]}{\delta \mathcal{G}}$$

75. The general many-body problem

75.1 An integral equation for the 4-point function

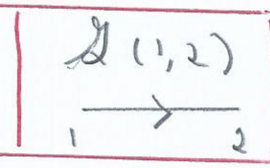
$$\frac{\delta}{\delta\varphi}\left(G^{-1}G\right) = 0$$

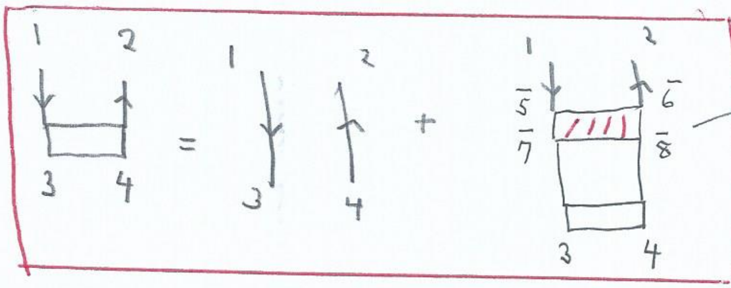
$$\frac{\delta G^{-1}}{\delta\varphi}G + G^{-1}\frac{\delta G}{\delta\varphi} = 0$$

$$\frac{\delta G}{\delta\varphi} = -G\,\frac{\delta G^{-1}}{\delta\varphi}\,G \qquad \text{but } G^{-1} = G_0^{-1} - \varphi - \Sigma$$

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

$$= G\,\frac{\delta\varphi}{\delta\varphi}\,G + G\left[\frac{\delta\Sigma}{\delta G}\,\frac{\delta G}{\delta\varphi}\right]G$$





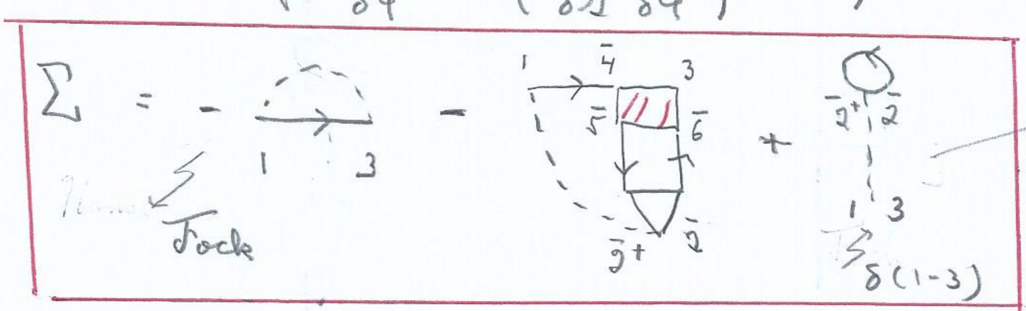
$\dfrac{\delta\Sigma(\bar{5},\bar{6})}{\delta G(\bar{7},\bar{8})}$ irreducible particle-hole vertex

75.2 Self-energy from functional derivative

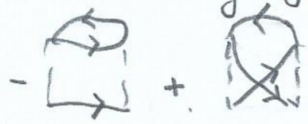
$$\Sigma = -V\left(\frac{\delta G}{\delta\varphi} - GG\right)G^{-1} \qquad \text{N.B.}\ \frac{}{\delta\varphi(\bar{2}^+,\bar{2})}\ V(1-\bar{2})$$

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

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



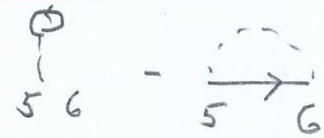
2^{nd} order perturbation theory by computing $\dfrac{\delta\Sigma}{\delta G}$ with

Hartree-Fock:  (see IPT)

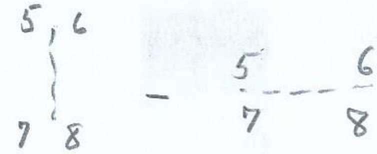
76. Long-range forces and GW

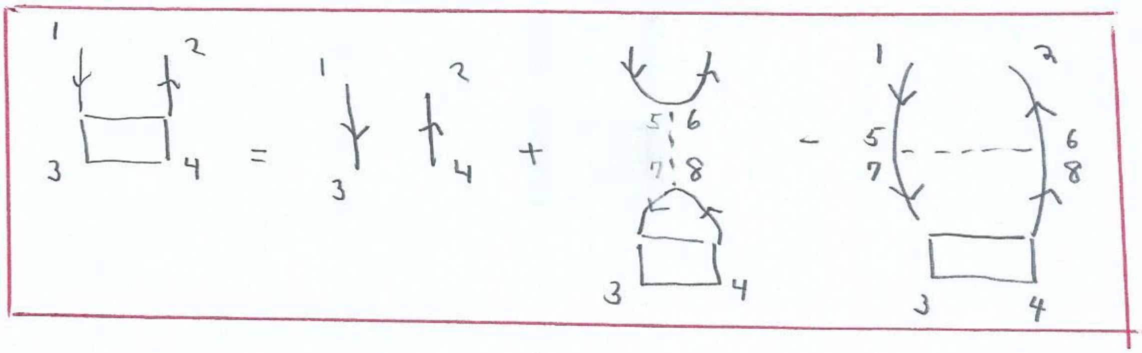
76.1 In space-time

$\Sigma(5,6) =$

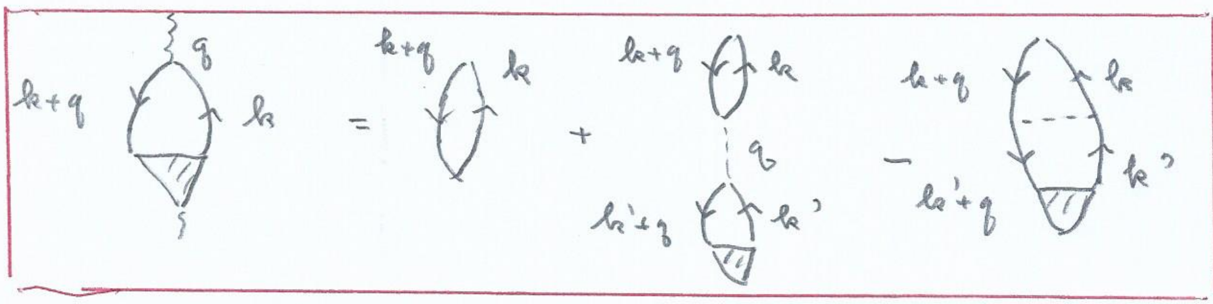


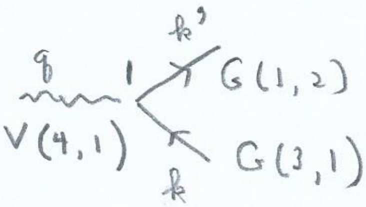
$$\frac{\delta \Sigma(5,6)}{\delta \mathcal{G}(7,8)} =$$





68.2 In momentum space with $\varphi=0$





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

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

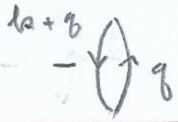
Conservation of 4-momentum at every vertex

76.3 Density response in the RPA

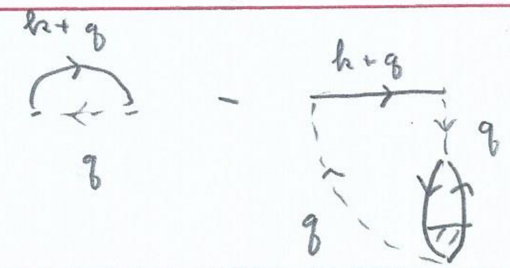
$$\chi_{nn}(1-2) = -\sum_{\sigma_1\sigma_2} \frac{\delta \mathcal{G}(1,1^+)}{\delta \phi(2^+,2)}$$

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

$$\chi_{nn}(q) = \frac{\chi^0_{nn}(q)}{1+V_q\chi^0_{nn}}$$ keeping the most divergent terms

$\chi^0_{nn}(q) = -$  Lindhard function

73.4 Σ and screening in the GW approximation

$\Sigma = -$ 

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

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

49. The Hubbard model in the foot steps of the electron gas

49.2 Response functions:

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

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

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

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

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

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

49.3 Hartree-Fock and RPA

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

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

$$\chi_{\substack{sp\\ch}} = \frac{\chi^0}{1 \mp \frac{U}{2}\chi^0}$$

$$\chi^0(1,2) = 2\mathcal{G}^H(1,2)\mathcal{G}^H(2,1)$$

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

Best numerically

Lindhard function

$$\chi^0 = -\frac{2}{N}\sum_{\vec{k}} \frac{f(\xi_{\vec{k}}) - f(\xi_{\vec{k}+\vec{q}})}{i\omega_n + \xi_{\vec{k}} - \xi_{\vec{k}+\vec{q}}}$$

49.4 RPA and the violation of the Pauli principle

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

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

$$\frac{T}{N}\sum_{q,iq_n}\left[\frac{\chi^0}{1-\frac{U}{2}\chi^0} + \frac{\chi^0}{1+\frac{U}{2}\chi_0}\right] \underset{O(U^2)}{\neq} 2\langle n\rangle - \langle n\rangle^2$$

49.6 RPA and the Mermin Wagner Theorem

$\chi^0 \propto N(0)\ln\left(\frac{E_F}{T}\right) \Rightarrow$ divergence at finite T

Mermin Wagner $\boxed{\langle S_z^2\rangle = \int d^2q\,\frac{k_BT}{q^2} = \infty}$ $\quad q^2\langle S_z(q)S_z(-q)\rangle = k_BT$

50. Two-Particle self-consistent

50.1 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 $2=1^+$ $\quad \Sigma^{(1)}_\sigma \mathcal{G}^{(1)}_\sigma = U\langle n_\uparrow n_\downarrow\rangle$

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

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

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

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

50.2 An improved self-energy

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

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

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

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

Do the same in the transverse channel

Assume crossing symmetry $\Rightarrow$

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

50.3 TPSC Internal accuracy check

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

Exact: $\frac{1}{2}\mathrm{Tr}[\Sigma^{(2)}\mathcal{G}^{(1)}] = U\langle n_\uparrow n_\downarrow\rangle$; $\frac{1}{2}\mathrm{Tr}[\Sigma^{(2)}\mathcal{G}^{(2)}] \overset{?}{=} U\langle n_\uparrow n_\downarrow\rangle$

accuracy check.