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École d'été 2016

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A1. Density matrix (used DMRG)

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

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

"pure" if $\rho^2 = \rho$ $\qquad \mathrm{Tr}[\rho] = 1$

A2. Statistical mechanics:

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

$$\rho = \sum_n |n\rangle \frac{e^{-\beta(E_n-\mu N_n)}}{Z} \langle n| = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{Z}$$

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

$$= \frac{\langle E - \mu N\rangle - \Omega}{T} \qquad \boxed{\Omega = -k_B T\, \mathrm{Tr}[\rho \ln Z]}$$
$$= -k_B T \ln Z$$

A3. Legendre transforms: (Self-energy functional)

$$dE = T\,dS - p\,dV \qquad T = \left(\frac{\partial E}{\partial S}\right)_V \qquad p = -\left(\frac{\partial E}{\partial V}\right)_S$$

$$F(T,V) = E(S(T,V),V) - T\,S(T,V)$$

where $S(T,V)$ obtained from $T(S,V) = \left(\frac{\partial E(S,V)}{\partial S}\right)_V$

$$dF = -S\,dT - p\,dV \qquad S = -\left(\frac{\partial F}{\partial T}\right)_V \qquad p = -\left(\frac{\partial F}{\partial V}\right)_T$$

Note the difference in formula for p depending on whether T or S is kept constant.
This accounts for changes in the energy of the bath at constant T.

59. Second quatization

59.1 States

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

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
- Works if interchange any two in the list

Annihilation:

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

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

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

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

Can construct number operator

$$\hat{n}_\alpha \equiv a^+_\alpha a_\alpha \qquad \boxed{n_\alpha a^+_\beta = a^+_\beta n_\alpha \text{ thanks to (1), (2)}}$$

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

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

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

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

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

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

59.2 Unitary change of basis

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

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

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

59.2.1 Position, momentum basis

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

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

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

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

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

59.3 One-body operators

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

in diagonal basis.

Example: (first quantized)

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

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

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

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

59.4 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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60.1 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

61. 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

62. Green functions contain useful information

Results of experiment related to correlation functions

62.1 Photoemission and fermion correlation function

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

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

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

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

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

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

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

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

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

62.2 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

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

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

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

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

62.3 Matsubara frequency representation is convenient

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

Proof: Let $\tau > 0$, then

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

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

Using the theorem on Fourier series

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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62.5 Spectral weight, relation to photoemission

62.6 Analytical continuation

63. Self-energy and the effect of interactions

63.1 The atomic limit

63.2 Self-energy and atomic limit

Dyson's equation

63.3 A few properties

63.4 Anderson impurity problem

62.5 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

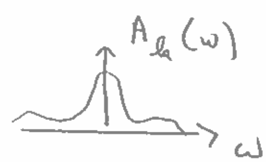
$$\boxed{\mathcal{G}(ik_n) = \int \frac{d\omega}{2\pi}\, \frac{A_k(\omega)}{ik_n-\omega}}$$

$A_k(\omega)$ = 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 $\Rightarrow$

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

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

Photoemission:

Photoemission:

We also have

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

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

62.6 $A_k(\omega)$ from $\mathcal{G}$: analytical continuation

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

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

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

63. Self-energy and the effect of interactions

63.1 The atomic limit $t=0$

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

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

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

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

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

$$+ \frac{e^{\beta(2\mu - U)}}{Z}(1 + e^{\beta\omega})\, 2\pi\, \delta(\omega - ((U - 2\mu) + \mu)) \quad \begin{cases} |m\rangle = |\uparrow\downarrow\rangle \\ |n\rangle = |\downarrow\rangle \end{cases}$$

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

$$+ \frac{e^{\beta(3\mu - U)} + e^{\beta\mu}}{Z}\, 2\pi\, \delta(\omega + \mu - U)$$

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

Alternatively

63. Self-energy and the effect of interactions

63.1 The atomic limit, $t=0$

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

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

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

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

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

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

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

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

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

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

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

63. 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

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

Dyson's equation:

In the non-interacting case:

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

Hence:

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

or:

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

63.3 A few properties:

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

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

63.4 "Integrating out the bath": Anderson impurity

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

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

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

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

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

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

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

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

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

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:

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

$\boxed{\#4}$

70. or 57. Coherent state for fermions

70.1 or 57.1 Fermion coherent states

57.2 Grassman calculus

57.3 Change of variables

57.4 Grassmann Gaussian integrals

57.5 Closure and Trace formula

58. Coherent state functional integral for fermions

58.1, 58.2 Single fermion without interactions

58.3 Wick's theorem

58.5 Effective action for quantum impurity

Hybridization expansion

70, or 57 Coherent state functional integrals

70.1 or 57.1 Fermion coherent states

$c|\eta\rangle = \eta|\eta\rangle$ by analogy with bosons, eigenstate of the destruction 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_2)

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

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

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

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

70.2 or 57.2 Grassman calculus

All functions are at most first order in η

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

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

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

57.3 Change of variables

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

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

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

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

57.4 Grassman Gaussian integrals

$$\int d\eta^+ \int d\eta_1\, e^{-\eta^+ a \eta} = \int d\eta^+ \int d\eta\, (1 - \eta^+ a \eta) = a$$

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

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

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

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

Source field: (J is a Grassman variable)

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

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

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

57.5 Trace for an operator with even # of fermions

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

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

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

$$= \langle 0 | O | 0 \rangle + \langle 1 | O | 1 \rangle$$

58. Coherent state functional integral for fermions

58.1 - 58.2 Fermion without interaction

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

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

Hence, in Matsubara basis:

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

58.3 Wick's theorem

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

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

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 $\mathcal{G}$.

58.5 Effective action for quantum impurity

$f \to \psi$

$c \to \eta$

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

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

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

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

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

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

Drops out from observables

See remark 205 in the notes for subtleties.

In the diagonal basis,

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

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

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,

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

$$\langle f^+(\tau_1') f(\tau_1) f^+(\tau_2') f(\tau_2) \ldots f^+(\tau_k') f(\tau_k) \rangle_{H_I}$$

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

#5

Iterated perturbation theory solver for DMFT

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 anticommutator.

Expanding $\dfrac{1}{ik_n+\mu-\epsilon_k-\Sigma(ik_n)} = G_k(ik_n)$

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

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

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)

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

  L.F. Arsenault et al. PRB 86 085133 (2012)

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

65. Source field to calculate many-body Green functions

65.1 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.

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

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

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

From the denominator

In particular, this is a way to compute correlation functions at $h = 0$

65.2 Green functions and higher order correlation functions

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

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

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

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

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

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

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

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

66.1 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

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

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

$$\boxed{\begin{gathered}\left[\mathcal{G}_0^{-1}(1,\bar{2}) - \varphi(1,\bar{2}) - \Sigma(1,\bar{2})_\varphi\right]\mathcal{G}(\bar{2},2)_\varphi = \delta(1,2) \\ \Sigma(1,\bar{2})_\varphi\, \mathcal{G}(\bar{2},2)_\varphi = -\langle T_\tau\left[\psi^+(\bar{2}^+)\,\psi(\bar{2})\,V(1-\bar{2})\,\psi_1\, \psi^+(2)\right]\rangle_\varphi\end{gathered}}$$

67. The general many-body problem

67.1 An integral equation for the 4-point function

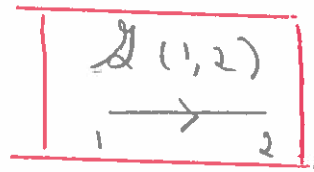
$$\frac{\delta}{\delta\varphi}\left(\mathcal{G}^{-1}\mathcal{G}\right)=0$$

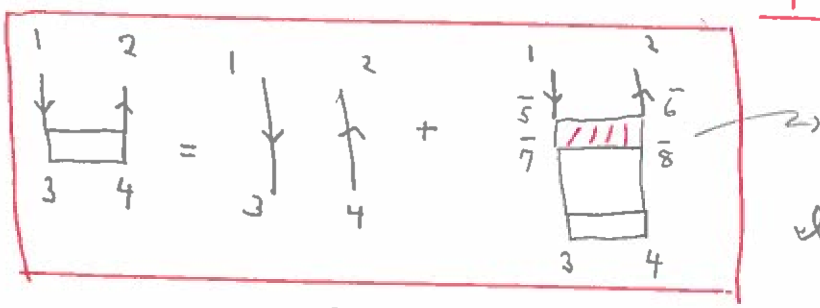
$$\frac{\delta\mathcal{G}^{-1}}{\delta\varphi}\mathcal{G}+\mathcal{G}^{-1}\frac{\delta\mathcal{G}}{\delta\varphi}=0$$

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

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

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





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

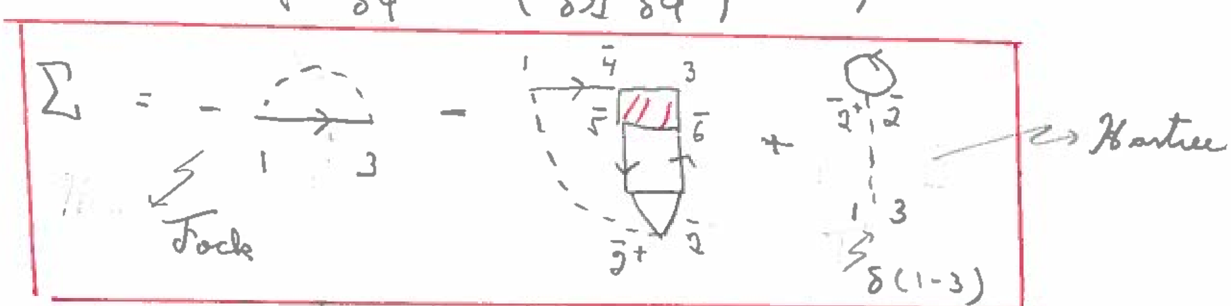
irreducible particle-hole vertex

67.2 Self-energy from functional derivative

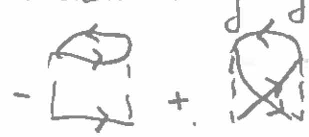
$$\Sigma=-V\left(\frac{\delta\mathcal{G}}{\delta\varphi}-\mathcal{G}\mathcal{G}\right)\mathcal{G}^{-1} \qquad \text{N.B. } \frac{}{\delta\varphi(\bar{2}^+,\bar{2})}\, V(1-\bar{2})$$

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

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

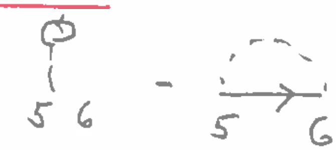


2^{nd} order perturbation theory by computing $\frac{\delta\Sigma}{\delta\mathcal{G}}$ with

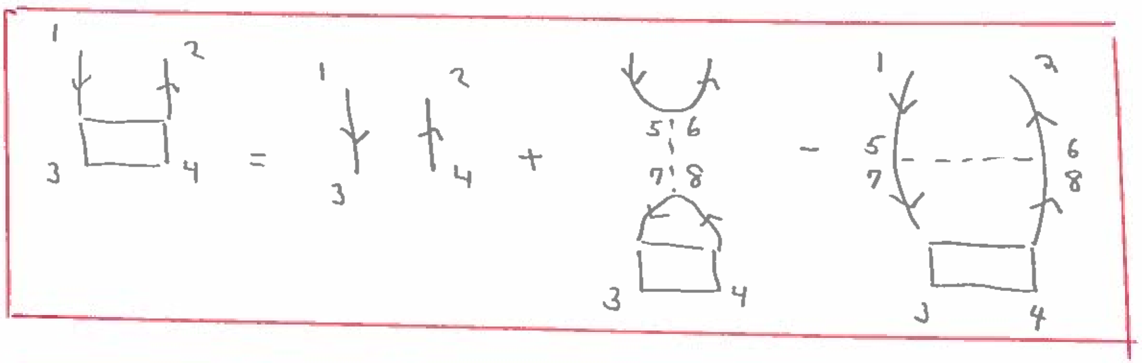
Hartree-Fock:  (see IPT)

68. Long-range forces and GW

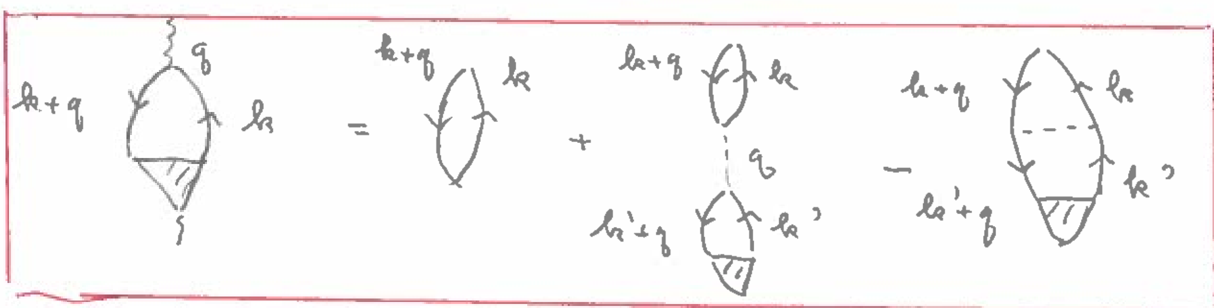
68.1 In space-time

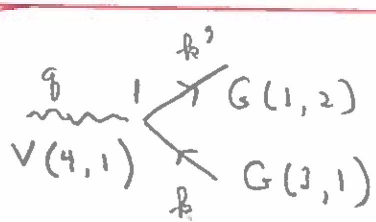
$\Sigma(5,6) =$ 

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



68.2 In momentum space with $\varphi = 0$





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

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

Conservation of 4-momentum at every vertex

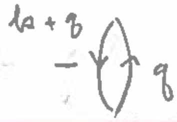
68.3 Density response in the RPA

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

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

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

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

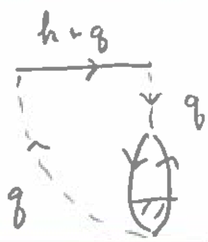


Lindhard function

68.4 Σ and screening in the GW approximation

$\Sigma = -$

$-$



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

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

69. Luttinger-Ward and related functionals

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

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

Legendre transform (assumes at least locally convex...)

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

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

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

"Integrating" from the equations of motion

$$\boxed{\begin{aligned}\Omega[\mathcal{G}] &= \mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_0}\right)\right] - \mathrm{Tr}\left[(\mathcal{G}_0^{-1} - \mathcal{G}^{-1})\mathcal{G}\right] + \Phi[\mathcal{G}] \\ &\text{where } \frac{1}{T}\frac{\delta\Phi}{\delta\mathcal{G}(1,2)} = \Sigma(2,1)\end{aligned}}$$

$\Omega[\mathcal{G}]$ correct limit when $\mathcal{G} = \mathcal{G}_0$

$\Phi[\mathcal{G}]$ Luttinger-Ward functional: contains the effects of interactions

We can find $\Phi[\mathcal{G}]$ as a universal functional of interactions from:

$$\frac{\partial \Omega_\lambda[\mathcal{G}]}{\partial \lambda}\bigg|_{\mathcal{G}} = \frac{\partial F_\lambda[q]}{\partial \lambda}\bigg|_{q} = \frac{\partial \Phi_\lambda[\mathcal{G}]}{\partial \lambda}\bigg|_{\mathcal{G}}$$

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

if we let the coupling constant take an arbitrary value.

Coupling constant integration

Potthoff functional

Let $\mathcal{G}^{-1} \equiv \mathcal{G}_0^{-1} - \Sigma$ with Σ that is varied instead of $\mathcal{G}$:

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

This is the only place where the non-interacting Hamiltonian appears.

Legendre transform of Φ. This is a universal functional of the interaction.