Many-body Green function (review)

N.B. (derivations in these notes are not rigorous)

Destruction operators $c_{k\sigma}|0\rangle = 0$

Antisymmetric states (Slater determinants)

$c^+_{k_1\sigma_1} c^+_{k_2\sigma_2} |0\rangle$ with anticommutation relations

(1) Let $K \equiv H - \mu N$

(2) Grand canonical averages: $\langle O \rangle = \dfrac{\mathrm{Tr}\, e^{-\beta K} O}{\mathrm{Tr}\, e^{-\beta K}}$, $Z \equiv \mathrm{Tr}\, e^{-\beta K}$

(3) Heisenberg equation of motion: $c_k(\tau) = e^{K\tau} c_{k\sigma} e^{-K\tau}$

($\hbar = 1$, τ is imaginary time for convenience)

Define Green function (Contains info. on one-particle properties)

(4) $G_\sigma(k,\tau) = -\langle c_{k\sigma}(\tau) c^+_{k\sigma} \rangle \theta(\tau) + \langle c^+_{k\sigma} c_{k\sigma}(\tau) \rangle \theta(-\tau)$

$$\theta(\tau) = \begin{cases} 1 & \tau > 0 \\ 0 & \tau < 0 \end{cases}$$

$$\equiv -\langle T_\tau\, c_{k\sigma}(\tau)\, c^+_{k\sigma} \rangle$$

T_τ: Time-ordered product

Special case: $G_\sigma(k, \tau = 0^-) = \langle n_{k\sigma} \rangle$

Antiperiodicity. Using cyclic property of trace it is easy to prove that

(5) $\tau < 0 \quad G_\sigma(k, \tau + \beta) = -G_\sigma(k, \tau)$

(6) $\tau > 0 \quad G_\sigma(k, \tau - \beta) = -G_\sigma(k, \tau)$

so that we can extend periodically beyond interval $-\beta < \tau \leq \beta$ and use Fourier series

$$(7) \quad G_\sigma(k, ik_n) = T \sum_{n=-\infty}^{\infty} e^{-ik_n\tau} G(k, ik_n)$$

$$(8) \quad k_n \equiv (2n+1)\pi\beta^{-1}$$ are "Matsubara" frequencies

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Example of non-interacting electrons

$$(9) \quad K_0 \equiv \sum_k (\epsilon_k - \mu)\, c^\dagger_{k\sigma} c_{k\sigma}$$

$$(10) \quad \frac{\partial c_{k\sigma}}{\partial \tau} = [K_0, c_{k\sigma}] = (\epsilon_k - \mu)\, c_{k\sigma}$$

$$(11) \quad \frac{\partial G^0_{k\sigma}(\tau)}{\partial \tau} = (\epsilon_k - \mu)\, G_{k\sigma} - \delta(\tau)$$

where we used $\{c_{k\sigma}, c^\dagger_{k\sigma}\} = 1$

Using Matsubara representation:

$$(12) \quad G^0_\sigma(k, ik_n) = \frac{1}{ik_n - (\epsilon_k - \mu)}$$

Or,

$$(13) \quad \left(G^0_\sigma(k, \tau - \tau')\right)^{-1} \equiv \left(\frac{\partial}{\partial \tau} - (\epsilon_k - \mu)\right)\delta(\tau - \tau')$$

$$(14) \quad \left(G^0_\sigma(\tau - \tau')\right)^{-1} G^0_\sigma(\tau' - \tau'') = \delta(\tau - \tau'')$$

Interpret matrix mult.
as integral over τ'

The Green function in the presence of source fields:

$$(15)\quad Z[\varphi] = \mathrm{Tr}\left[e^{-\beta K} \, T_\tau \, e^{-\psi_\sigma^+(\bar{1})\,\varphi_\sigma(\bar{1},\bar{2})\,\psi_\sigma(\bar{2})} \right]$$

where $\varphi_\sigma(1,2)$ is the source field

and $1 \equiv (\vec{r}_1, \tau_1)$

$$\bar{1} \longrightarrow \int_0^\beta d\tau_1 \sum_{\vec{r}_1}$$

in other words, the overbar means integrate over τ_1 and sum over spatial indices

In this notation, it is possible to have $1 = 2$.

Then

$$(16)\quad G_\sigma(1,2;\varphi) = -\frac{\delta \ln Z}{\delta \varphi(2,1)} = -\langle \psi(1)\,\psi^+(2) \rangle$$

From now on it is implicit that we work with time-ordered products when we write $\langle \ \ \rangle$

Using Heisenberg equations of motion to evaluate $\frac{\partial}{\partial \tau}$, we find,

$$(17)\quad (G_0^{-1} - \varphi)\,G = (1 + \Sigma G) \Longrightarrow G^{-1} = G_0^{-1} - \varphi - \Sigma$$

where ΣG simply comes from commutator with interaction, i.e. it is defined as,

$$(18)\quad \Sigma_\sigma(1,\bar{1})\,G_\sigma(\bar{1},2) = -U\langle \psi_{-\sigma}^+(1^+)\,\psi_{-\sigma}(1)\,\psi_\sigma(1)\,\psi_\sigma^+(2) \rangle$$

Response functions $\qquad$ $(1^+ \Rightarrow \tau_1 + 0^+$ so that

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(19) $\quad G G^{-1} = 1$

(20) $\quad \dfrac{\delta G}{\delta \varphi} G^{-1} + G \dfrac{\delta G^{-1}}{\delta \varphi} = 0$

(21) $\quad \dfrac{\delta G}{\delta \varphi} = - G \dfrac{\delta G^{-1}}{\delta \varphi} G$

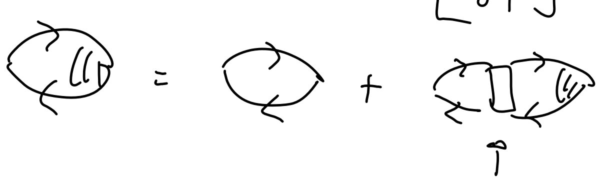
and since $G^{-1} = G_0^{-1} - \varphi - \Sigma$

$$= G_\Lambda G + G \frac{\delta \Sigma}{\delta \varphi} G$$

But Σ can be written as a functional of G (see Potthoff for general proof)

(22) $\quad \dfrac{\delta G}{\delta \varphi} = G_\Lambda G + G \left[\dfrac{\delta \Sigma}{\delta G} \dfrac{\delta G}{\delta \varphi} \right] G$

$$= G_\Lambda G + G \left[\begin{array}{c} \dfrac{\delta \Sigma}{\delta G} \\ \dfrac{\delta G}{\delta \varphi} \end{array} \right] G$$



$\dfrac{\delta \Sigma}{\delta G}$ = irreducible vertex

For spin and charge fluctuations, we must take symmetric and anti-symmetric spin combinations so,

(23) $\quad \Gamma_{sp} = \dfrac{\delta \Sigma_\uparrow}{\delta G_\downarrow} - \dfrac{\delta \Sigma_\uparrow}{\delta G_\uparrow} \;;\; \Gamma_{ch} = \dfrac{\delta \Sigma_\uparrow}{\delta G_\downarrow} + \dfrac{\delta \Sigma_\uparrow}{\delta G_\uparrow}$

JPSC

Step 1: Note that (consistency between one- and two-ptcle)

(24) $\Sigma_\sigma^{(1)}(1,\bar{1})\, G_\sigma^{(1)}(\bar{1},1^+) = U\langle n_\uparrow n_\downarrow\rangle$ (exact)

In general, factor the 4-pt function entering the equs. of motion "à la Hartree-Fock" but such that (24) is satisfied exactly. Then (18) becomes

$$(25)\quad \Sigma_\sigma^{(1)}(1,\bar{1})\, G_\sigma^{(1)}(\bar{1},2) = U_{sp}\, G_{-\sigma}^{(1)}(1,1^+)\, G_\sigma^{(1)}(1,2)$$

Comparing with (24), since $G_{-\sigma}^{(1)}(1,1^+) = \langle n_{-\sigma}\rangle$ we have

$$(26)\quad \boxed{U_{sp} \equiv \frac{U\langle n_\uparrow n_\downarrow\rangle}{\langle n_\uparrow\rangle\langle n_\downarrow\rangle}}$$

Multiply by $\left(G^{(1)}\right)^{-1}$ from the right $\Rightarrow$

$$(27)\quad \Sigma_\sigma^{(1)}(1,2) = U_{sp}\, G_{-\sigma}^{(1)}(1,1^+)\,\delta(1-2)$$

so that + terme

$$(28)\quad \frac{\delta\Sigma_\sigma^{(1)}(1,2)}{\delta G_{-\sigma}^{(1)}(3\ 4)} = U_{sp}\,\delta(1-2)\,\delta(3-1)\,\delta(4-2)$$

+ terms that involve $\dfrac{\delta U_{sp}}{\delta G_{-\sigma}^{(1)}}$

In computing Γ_{sp} with (23) that last term simplifies by symmetry and

$$(29)\quad \Gamma_{sp} = U_{sp}$$

Substituting back in Bethe-Salpeter equation

$$(30)\quad \chi_{sp}(q) = \chi_0(q) + \chi_0(q)\,\frac{U_{sp}}{2}\,\chi_{sp}(q)$$

$$(31)\quad q \equiv (\vec{q}, iq_n) \qquad q_n = 2n\pi/\beta^{-1}$$

To close the system of equations, use the Pauli principle and the fluctuation-dissipation theorem:

(32) $\langle (n_\uparrow - n_\downarrow)(n_\uparrow - n_\downarrow)\rangle = \langle n_\uparrow\rangle + \langle n_\downarrow\rangle - 2\langle n_\uparrow n_\downarrow\rangle$

same space-time point

since $n_\uparrow^2 = n_\uparrow$ for one band.

Since $\langle n_\uparrow\rangle + \langle n_\downarrow\rangle = n$,

(33) $$n - 2\langle n_\uparrow n_\downarrow\rangle = \frac{T}{N}\sum_q \frac{\chi_0(q)}{1 - \frac{U_{sp}}{2}\chi_0(q)}$$

which, using (23), gives a closed set of equations, for $\langle n_\uparrow n_\downarrow\rangle$.

Assuming Γ_{ch} is also local, we have

(34) $$n + 2\langle n_\uparrow n_\downarrow\rangle - n^2 = \frac{T}{N}\sum_q \frac{\chi_0(q)}{1 + \frac{U_{ch}}{2}\chi_0(q)}$$

Must subtract disconnected part

- Mermin-Wagner automatically satisfied
- as well as Pauli
- U_{sp} is renormalized clearly (Kanamori-Brueckner)

<u>Step 2</u>: improve the self-energy

Given the general formula (18)

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

(Must be subtracted because $\frac{\delta}{\delta\varphi}Z^{-1}$ generates unwanted term)

Multiply by G^{-1} from the right.

(36) $$\Sigma_\sigma(1,2) = U\,G_{-\sigma}(1,1^+)\,\delta(1-2) - U\,\frac{\delta G}{\delta\varphi}G^{-1}$$

$$= U\,G_{-\sigma}(1,1^+)\,\delta(1-2) + U\,G_\sigma\frac{\delta G_\sigma^{-1}}{\delta\varphi_{-\sigma}}$$

$$= U\, G_{-\sigma}(1,1^+)\,\delta(1-2) + U\, G_\sigma \frac{\delta G_\sigma^{-1}}{\delta \varphi_{-\sigma}}$$

G_σ^{-1} has no explicit dep. on $\varphi_{-\sigma}$ $\Rightarrow$

$$= U\, G_{-\sigma}(1,1^+)\,\delta(1-2) + U\, G_\sigma \frac{\delta \Sigma_\sigma}{\delta \varphi_{-\sigma}}$$

$$= U\, G_{-\sigma}(1,1^+)\,\delta(1-2) + U\, G_\sigma \frac{\delta \Sigma_\sigma}{\delta G_{\sigma'}} \frac{\delta G_{\sigma'}}{\delta \varphi_{-\sigma}}$$

irreducible vertex.

- Replace everything to the right by what we obtained at first step. Then

$$(37) \quad \Sigma_\sigma^{(2)} G_\sigma^{(1)} = U \langle n_\uparrow n_\downarrow \rangle$$

is garanteeded. Then check quality of approximation by

$$(38) \quad \Sigma_\sigma^{(2)} G_\sigma^{(2)} \cong U \langle n_\uparrow n_\downarrow \rangle$$

Rederive analog formula in transverse channel and insist on crossing symmetry $\Rightarrow$

$$(39) \quad \Sigma^{(2)}(k, ik_n) = U n_{-\sigma}$$

$$+ \frac{T}{4N} U \sum_q \left[\frac{3}{2} U_{sp} \chi_{sp}(q) + \frac{1}{2} U_{ch} \chi_{ch}(q) \right] G(k+q)$$

CDMFT as special case of Self-Energy functional theory

(40) $\Omega[\varphi] = -T \ln Z[\varphi]$ is the grand-potential at $\varphi = 0$ ($k_B = 1$)

From (15):

(41) $\frac{1}{T} \frac{\delta \Omega}{\delta \varphi(1,2)} = G(2,1)$ (note inverted indices as usual)

Define $\mathrm{Tr}\, A = T \sum_{iq_n} \sum_{\alpha} A_{\alpha\alpha}(iq_n)$

Then, the Legendre transform

(42) $\tilde{\Omega}[G] = \Omega[\varphi] - \mathrm{Tr}[\varphi G]$

is equal to the grand potential at $\varphi = 0$ and satisfies:

(43) $\frac{1}{T} \frac{\delta \tilde{\Omega}}{\delta G} = -\varphi = G^{-1} - G_0^{-1} + \Sigma$

Follows from (17)

So when the usual Dyson equation is satisfied at $\varphi = 0$, then $\tilde{\Omega} = \Omega$ is the grand potential

Now we can guess that

(44) $\tilde{\Omega}[G] = \Phi[G] - \mathrm{Tr}\left((G_0^{-1} - G^{-1})G\right) + \mathrm{Tr} \ln(-G)$

where (45) $\frac{1}{T} \frac{\delta \Phi}{\delta G} = \Sigma$

Φ is the Luttinger-Ward functional

It is easy to check from (45) and (44) that we obtain (43). Also, check that correct answer at $U = 0$ (No integ. constant).

we obtain (43). Also, check that correct answer at $U=0$ (No integ. constant).

$\tilde{\Omega}[G]$ equals the grand potential at the stationnary pt where Dyson equation is satisfied.

Use (45) to solve for $G[\Sigma]$ and, inspired by (44), write a new functional,

$$(45) \quad \tilde{\Omega}[G[\Sigma]] = \Phi[G[\Sigma]] - \mathrm{Tr}[\Sigma G[\Sigma]] - \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma))$$

$$(46) \quad \tilde{\Omega}_t[\Sigma] \equiv F[\Sigma] - \mathrm{Tr}\ln(-(G_{0t}^{-1} - \Sigma))$$

where the one-body Hamiltonian (parametrized by matrix t) occurs only in G_{0t}^{-1}

and where $F[\Sigma]$ is the Legendre transform of Φ.

$$(47) \quad \frac{1}{T}\frac{\delta F[\Sigma]}{\delta \Sigma} = -G$$

Φ depends only on the form of the interaction.

As a functional of G $\left(= U\int GG + U^2\int GGGG + \ldots\right)$ it is independent of the explicit form of H_0, it depends only on the form of the interaction.

Potthoff's classification of approximations:

Type I : approximate the Euler equation

Type II : Take a few diagrams for Φ

Type III : Evaluate the exact functional, but only in a restricted subspace.

Following Type III, take a one-body Hamiltonian t' that decomposes the infinite lattice into a set of solvable clusters. Then,

$$F[\Sigma_{t'}] = \tilde{\Omega}_{t'}[\Sigma_{t'}] + \mathrm{Tr}\ln\left(-(G_{0\,t'}^{-1} - \Sigma_{t'})\right) \tag{48}$$

These are "t' representable".

The r.h.s. is obtained from exact solution.

Note that $F[\Sigma_{t'}]$ is exact but Σ can be varied only by changing t' (that can contain "Bath" terms)

We thus approximate,

$$\tilde{\Omega}_{t}[\Sigma_{t'}] = F[\Sigma_{t'}] - \mathrm{Tr}\ln\left(-(G_{0\,t}^{-1} - \Sigma_{t'})\right) \tag{49}$$

"Self-energy of the lattice = cluster's"

Varying t':

$$\frac{\partial \tilde{\Omega}_t}{\partial t'} = \left(\cancel{\frac{\partial \tilde{\Omega}_{t'}}{\partial t'}} + \mathrm{Tr}\left(\frac{1}{G_{0\,t'}^{-1} - \Sigma_{t'}} \left(\cancel{\frac{\partial G_{0\,t'}^{-1}}{\partial t'}} - \frac{\partial \Sigma_{t'}}{\partial t'} \right) \right) \right) \tag{50}$$

$$+ \mathrm{Tr}\left[\frac{1}{G_{0\,t}^{-1} - \Sigma_{t'}} \frac{\partial \Sigma_{t'}}{\partial t'} \right] = 0$$

The terms marked 1 disappear because for an exact solution, the one-body terms obtained from a derivative of the grand potential are equal to those calculated with the one-body Green function. We are thus left with,

$$\mathrm{Tr}\left[\left(\frac{1}{G_{0\,t'}^{-1} - \Sigma_{t'}} - \frac{1}{G_{0\,t}^{-1} - \Sigma_{t'}} \right) \cdot \frac{\partial \Sigma_{t'}}{\partial t'} \right] = 0 \tag{51}$$

In practice, in VCPT (variational cluster perturbation theory) $\tilde{\Omega}_{t'}[\Sigma_{t'}]$ is directly minimized.

CDMFT consits in insisting that each component of the term in parenthesis vanishes on the cluster, i.e.

$$\frac{N}{N_c}\left(\frac{1}{G_{0\,t'}^{-1}-\Sigma_{t'}}\right)_{\mu\nu} = \sum_{\tilde{k}} \left[\frac{1}{i\omega_n-(\epsilon_{\tilde{k}}-\mu)-\Sigma_{t'}}\right]_{\mu\nu} \tag{52}$$

cluster indices

N = total number of sites
N_c = number of sites in a cluster

$\tilde{k}$ = vectors in the Brillouin zone (small) of the superlattice.

It is as if $\frac{\partial \Sigma_{t'}}{\partial t'}$ = constant and we evaluated the trace on the superlattice degrees of freedom.

The "periodized" Green function is obtained as in CPT:

$$G_\sigma(k, ik_n) =$$

$$= \sum_{\mu\nu} e^{-ik\cdot(r_\mu-r_\nu)} \left[\frac{1}{i\omega_n+\mu-\epsilon_{\tilde{k}}-\Sigma_{t'}}\right]_{\mu\nu} \tag{53}$$