

Lecture on First-principles Computations (21)

Introduction to the Green Function Theory

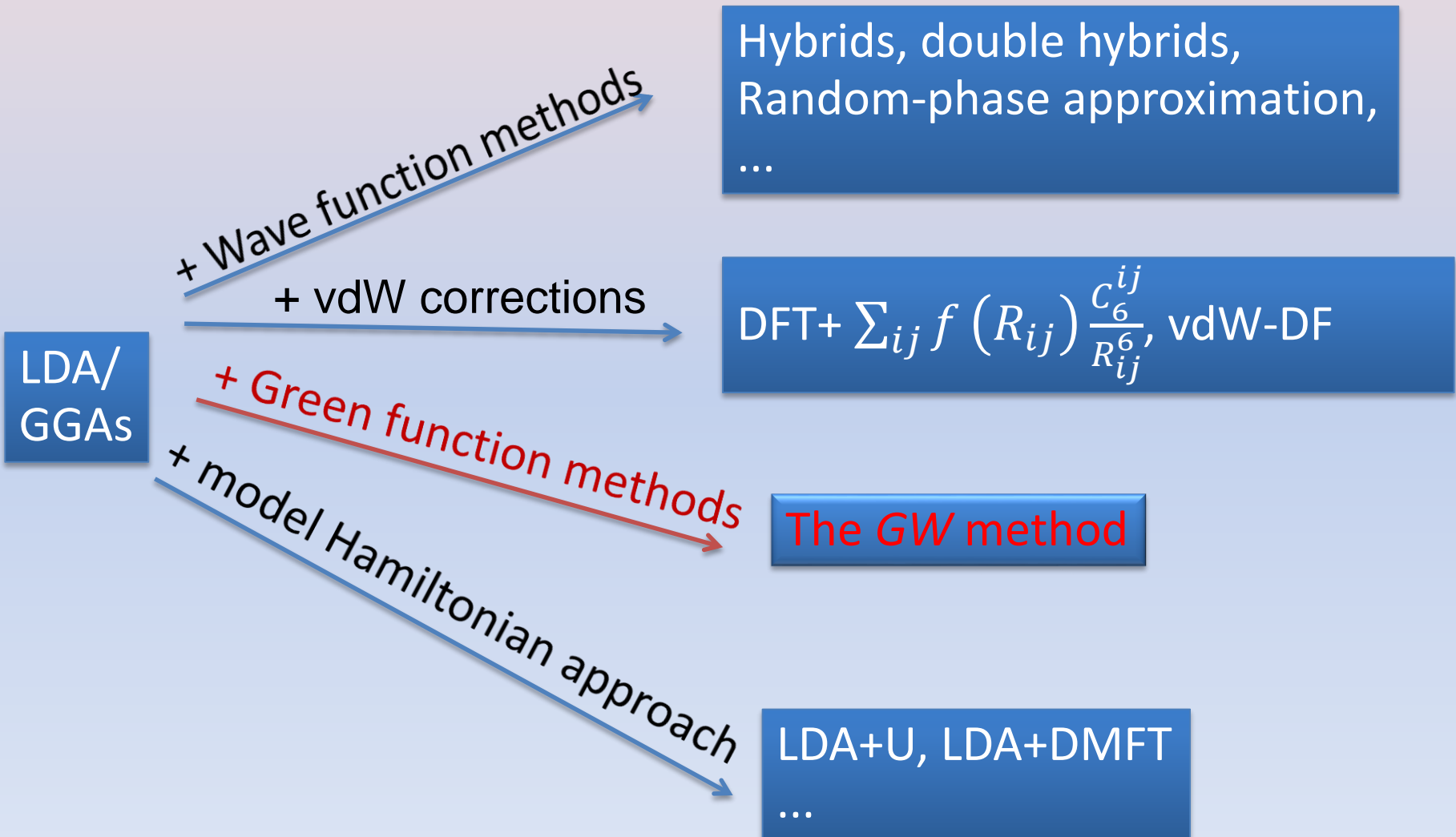
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Computational schemes beyond LDA and GGAs



Why bother?

- Green function is a useful quantity; **many physical observables can be directly obtained if Green function of the system is known.**

One-particle Green function →

1. the expectation value of any single-particle operator within the ground state of the system
 2. the ground-state energy
 3. **the excitation spectrum of the system**
- Many-body theories, which are required in in many situations, can be most conveniently expressed in terms of Green function
 - The Feynman rule for carrying out the many-body perturbation theory is simpler for Green function than for other quantities.

Second quantization for fermionic systems

Define an orthonormal single-particle orbital :

$$|i\rangle = |\phi_i\rangle, \quad i = 1, 2, \dots, M \quad (\text{ordered in certain way})$$

N -body ($N \leq M$) wave function can be expanded as :

$$\Psi(x_1, \dots, x_N, t) = \sum_{n_1, \dots, n_M=0}^1 f(n_1, \dots, n_M, t) \Phi_{n_1, \dots, n_M}(x_1, \dots, x_N)$$

$x = (\mathbf{r}, \sigma)$

$$\Phi_{n_1, \dots, n_M}(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{j_1}(x_1) & \dots & \phi_{j_1}(x_N) \\ \dots & \vdots & \dots \\ \phi_{j_N}(x_1) & \dots & \phi_{j_N}(x_N) \end{vmatrix} \quad (j_1 < j_2 < \dots < j_N)$$

Formally we can write

$$|\Psi(t)\rangle = \sum_{n_1, \dots, n_M} f(n_1, n_2, \dots, n_M, t) |n_1, n_2, \dots, n_M\rangle, \quad n_i = 0, 1$$

Second quantization for fermionic systems

$$|\Psi(t)\rangle = \sum_{n_1, \dots, n_M} f(n_1, n_2, \dots, n_M, t) |n_1, n_2, \dots, n_M\rangle, \quad n_i = 0, 1$$

Define creation and annihilation operators:

$$\hat{c}_k^\dagger |0\rangle_{k'} = \delta_{kk'} |1\rangle_k, \quad \hat{c}_k^\dagger |1\rangle_{k'} = 0; \quad \hat{c}_k |0\rangle_{k'} = 0, \quad \hat{c}_k |1\rangle_{k'} = \delta_{kk'} |0\rangle_{k'}$$

$$\hat{n}_k = \hat{c}_k^\dagger \hat{c}_k \quad : \text{Particle number operator}$$

The anti-commutation rule:

$$[\hat{c}_k, \hat{c}_{k'}^\dagger]_+ = \hat{c}_k \hat{c}_{k'}^\dagger + \hat{c}_{k'}^\dagger \hat{c}_k = \delta_{kk'}$$

$$[\hat{c}_k, \hat{c}_{k'}]_+ = [\hat{c}_k^\dagger, \hat{c}_{k'}^\dagger]_+ = 0$$

$$|n_1, n_2, \dots, n_M\rangle = (c_1^\dagger)^{n_1} (c_2^\dagger)^{n_2} \dots (c_M^\dagger)^{n_M} |Vaccum\rangle$$

$$\hat{n}_k |n_1, n_2, \dots, n_M\rangle = n_k |n_1, n_2, \dots, n_M\rangle$$

The operators in second-quantization representation

Single-particle operators:

$$\hat{Q} = \sum_{k=1}^N \hat{q}(x_k) \quad \text{e.g.,} \quad \hat{T} = - \sum_{k=1}^N \frac{\nabla_k^2}{2}$$

Under second quantization:

$$\hat{Q} = \sum_{ij} q_{ij} \hat{c}_i^\dagger \hat{c}_j, \quad q_{ij} = \langle i | \hat{q} | j \rangle$$

The Hamiltonian operator:

$$\hat{H} = \sum_{ij} h_{ij}^0 \hat{c}_i^\dagger \hat{c}_j + \frac{1}{2} \sum_{ijkl} V_{ijkl} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_l \hat{c}_k$$

$$V_{ijkl} = \langle ij | V | kl \rangle = \int \int d x_1 d x_2 \phi_i^*(x_1) \phi_j^*(x_2) V(x_1 - x_2) \phi_k(x_1) \phi_l(x_2)$$

The Field operators

$$\hat{\psi}^\dagger(x) = \sum_i \hat{c}_i^\dagger \phi_i^*(x); \quad \hat{\psi}(x) = \sum_i \hat{c}_i \phi_i(x)$$

Field operators are real-space representation of the creation and annihilation operators!

For fermions, the anti-commutation rule

$$[\hat{\psi}(x), \hat{\psi}^\dagger(x')]_+ = \delta(x - x')$$

$$[\hat{\psi}(x), \hat{\psi}(x')]_+ = [\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x')]_+ = 0$$

The density operator:

$$\hat{n}(x) = \hat{\psi}^\dagger(x)\hat{\psi}(x) \quad n(x) = \langle \Psi | \hat{\psi}^\dagger(x)\hat{\psi}(x) | \Psi \rangle / \langle \Psi | \Psi \rangle$$

The Hamiltonian operator:

$$\hat{H} = \int dx \hat{\psi}^\dagger(x) h^0(x) \hat{\psi}(x) + \frac{1}{2} \int \int dx dx' \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') V(x, x') \hat{\psi}(x') \hat{\psi}(x)$$

Schrödinger picture vs Heisenberg picture

Schrödinger picture:

$$i \frac{\partial |\Psi_S(t)\rangle}{\partial t} = \hat{H} |\Psi_S(t)\rangle$$

$$|\Psi_S(t)\rangle = e^{-i\hat{H}(t-t_0)} |\Psi_S(t_0)\rangle, \quad O(t) = \langle \Psi_S(t) | \hat{O}_S | \Psi_S(t) \rangle$$

Heisenberger Picture:

$$|\Psi_H(t)\rangle = e^{i\hat{H}t} |\Psi_S(t)\rangle, \quad i \frac{\partial |\Psi_H(t)\rangle}{\partial t} = 0$$

$$O(t) = \langle \Psi_H | \hat{O}_H(t) | \Psi_H \rangle, \quad \hat{O}_H(t) = e^{i\hat{H}t} \hat{O}_S e^{-i\hat{H}t}$$

$$\hat{H}_H(t) = \hat{H}_S = \hat{H}$$

Definition of the Green function

Time-ordered Green function:

$$G(x, t; x', t') = \frac{-i \langle \Psi_0 | T \hat{\psi}(x, t) \hat{\psi}^\dagger(x', t') | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

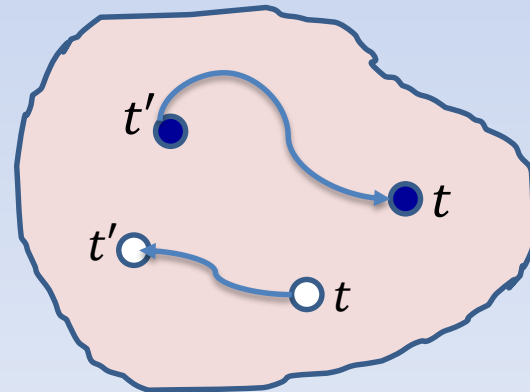
Time-ordered operator

Many-body ground state

$$T \hat{\psi}(x, t) \hat{\psi}^\dagger(x', t') = \begin{cases} \hat{\psi}(x, t) \hat{\psi}^\dagger(x', t'), & t > t' \\ -\hat{\psi}^\dagger(x', t') \hat{\psi}(x, t), & t < t' \end{cases}$$

Time-dependent field operator:

$$\hat{\psi}(x, t) = e^{i\hat{H}t} \hat{\psi}(x) e^{-i\hat{H}t}$$



One-particle properties from the Green function

$$G(x, t; x', t') = G(x, x'; t - t') =$$

$$\begin{cases} -ie^{iE_0(t-t')} \langle \Psi_0 | \hat{\Psi}(x) e^{-i\hat{H}(t-t')} \hat{\Psi}^\dagger(x') | \Psi_0 \rangle / \langle \Psi_0 | \Psi_0 \rangle, & t > t' \\ ie^{-iE_0(t-t')} \langle \Psi_0 | \hat{\Psi}^\dagger(x') e^{i\hat{H}(t-t')} \hat{\Psi}(x) | \Psi_0 \rangle / \langle \Psi_0 | \Psi_0 \rangle, & t < t' \end{cases}$$

Density matrix: $x = (\mathbf{r}, \sigma)$

$$\begin{aligned} \rho_\sigma(\mathbf{r}, \mathbf{r}') &= -i \lim_{t' \rightarrow t^+} G(\mathbf{r}, \sigma, t; \mathbf{r}', \sigma, t') = -i \lim_{t-t' \rightarrow 0^-} G(\mathbf{r}, \sigma; \mathbf{r}', \sigma; t - t') \\ &= -iG(\mathbf{r}, \sigma; \mathbf{r}', \sigma; 0^-) \end{aligned}$$

Spin-polarized electron density:

$$n_\sigma(\mathbf{r}) = \rho_\sigma(\mathbf{r}, \mathbf{r}) = G(\mathbf{r}, \sigma; \mathbf{r}, \sigma; 0^-)$$

The kinetic energy density:

$$\epsilon_k(\mathbf{r}) = -i \lim_{r' \rightarrow \mathbf{r}} \sum_{\sigma} \left(-\frac{\nabla_r^2}{2} \right) G(\mathbf{r}, \sigma; \mathbf{r}', \sigma; 0^-)$$

The ground-state energy

$$E_0 = \langle \hat{H} \rangle = \langle \hat{H}_0 \rangle + \langle \hat{V} \rangle$$

$$\hat{H} = \int dx \hat{\psi}^\dagger(x) h^0(x) \hat{\psi}(x) + \frac{1}{2} \int \int dx dx' \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') V(x, x') \hat{\psi}(x') \hat{\psi}(x)$$

$$\langle \hat{H}_0 \rangle = \int dx \langle \hat{\psi}^\dagger(x) h^0(x) \hat{\psi}(x) \rangle = -i \int dx \lim_{x' \rightarrow x} h^0(x) G(x, x'; 0^-)$$

$$\langle \hat{V} \rangle = \frac{1}{2} \int \int dx dx' V(x, x') \langle \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') \hat{\psi}(x') \hat{\psi}(x) \rangle$$

How to obtain the expectation value of the product of 4 fermion operators?

The key is the equation of motion of the Green function!

The Galitskii-Migdal formula

$$G(x, t; x', t') = -i \langle \Psi_0 | T \hat{\Psi}(x, t) \hat{\Psi}^\dagger(x', t') | \Psi_0 \rangle \quad (\text{assuming } \langle \Psi_0 | \Psi_0 \rangle = 0)$$

$$i \frac{\partial}{\partial t} G(x, t; x', t') = -i \langle \Psi_0 | T \left(i \frac{\partial}{\partial t} \hat{\Psi}(x, t) \right) \hat{\Psi}^\dagger(x', t') | \Psi_0 \rangle$$

$$i \frac{\partial}{\partial t} \hat{\Psi}(x, t) = [\hat{\Psi}(x, t), \hat{H}] = h_0(x) \hat{\Psi}(x, t) + \int dx' \hat{\Psi}^\dagger(x', t) V(x, x') \hat{\Psi}(x', t) \hat{\Psi}(x, t)$$

$$\Rightarrow \langle \hat{V} \rangle = -\frac{i}{2} \int dx \lim_{t' \rightarrow t^+} \lim_{x' \rightarrow x} \left(i \frac{\partial}{\partial t} - h_0(x) \right) G(x, t; x, t')$$

The Galitskii-Migdal formula

$$E_0 = \langle \hat{H}_0 \rangle + \langle \hat{V} \rangle = -\frac{i}{2} \int dx \lim_{t' \rightarrow t^+} \lim_{x' \rightarrow x} \left(i \frac{\partial}{\partial t} + h_0(x) \right) G(x, t; x, t')$$

The Lehmann representation

Variable replacement : $t - t' \rightarrow t$

$$G(x, x'; t) = -i\theta(t)\langle\Psi_0 | \hat{\Psi}(x, t)\hat{\Psi}^\dagger(x', 0) | \Psi_0\rangle \\ +i\theta(-t)\langle\Psi_0 | \hat{\Psi}^\dagger(x', 0)\hat{\Psi}(x, t) | \Psi_0\rangle$$

Denoting $|\Psi_0\rangle = |\Psi_0^N\rangle$ $\sum_s |\Psi_s^{N+1}\rangle\langle\Psi_s^{N+1}| = 1$, $\sum_r |\Psi_r^{N-1}\rangle\langle\Psi_r^{N-1}| = 1$

$$G(x, x'; t) = -i\theta(t) \sum_s \langle\Psi_0^N | \hat{\Psi}(x, t) | \Psi_s^{N+1}\rangle \langle\Psi_s^{N+1} | \hat{\Psi}^\dagger(x', 0) | \Psi_0\rangle \\ +i\theta(-t) \sum_r \langle\Psi_0^N | \hat{\Psi}^\dagger(x', 0) | \Psi_r^{N-1}\rangle \langle\Psi_r^{N-1} | \hat{\Psi}(x, t) | \Psi_0\rangle \\ = -i\theta(t) \sum_s e^{i(E_0^N - E_s^{N+1})t} \langle\Psi_0^N | \hat{\Psi}(x) | \Psi_s^{N+1}\rangle \langle\Psi_s^{N+1} | \hat{\Psi}^\dagger(x') | \Psi_0\rangle \\ +i\theta(-t) \sum_r e^{i(E_r^{N-1} - E_0^N)t} \langle\Psi_0^N | \hat{\Psi}^\dagger(x') | \Psi_r^{N-1}\rangle \langle\Psi_r^{N-1} | \hat{\Psi}(x) | \Psi_0\rangle$$

The Lehmann representation

$$G(x, x'; t) = -i\theta(t) \sum_s e^{i(E_0^N - E_s^{N+1})t} \langle \Psi_0^N | \hat{\Psi}(x) | \Psi_s^{N+1} \rangle \langle \Psi_s^{N+1} | \hat{\Psi}^\dagger(x') | \Psi_0 \rangle$$

$$+ i\theta(-t) \sum_r e^{i(E_r^{N-1} - E_0^N)t} \langle \Psi_0^N | \hat{\Psi}^\dagger(x') | \Psi_r^{N-1} \rangle \langle \Psi_r^{N-1} | \hat{\Psi}(x) | \Psi_0 \rangle$$

$$\theta(t) = - \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{e^{-i\omega t}}{\omega + i\eta}$$

$$G(x, x'; \omega) = \int_{-\infty}^{\infty} G(x, x'; t) e^{i\omega t} dt =$$

$$\sum_s \frac{\langle \Psi_0^N | \hat{\Psi}(x) | \Psi_s^{N+1} \rangle \langle \Psi_s^{N+1} | \hat{\Psi}^\dagger(x') | \Psi_0 \rangle}{\omega - (E_s^{N+1} - E_0^N) + i\eta} +$$

$$\sum_r \frac{\langle \Psi_0^N | \hat{\Psi}^\dagger(x') | \Psi_r^{N-1} \rangle \langle \Psi_r^{N-1} | \hat{\Psi}(x) | \Psi_0 \rangle}{\omega - (E_0^N - E_r^{N-1}) - i\eta}$$

Green function for non-interacting systems

The Hamiltonian:

$$\hat{H} = \hat{H}_0 + \hat{H}_{int} \quad \text{where} \quad \hat{H}_{int} = 0$$

$$\hat{H}_0 = \sum_n \epsilon_n \hat{c}_n^\dagger \hat{c}_n \quad \longrightarrow \quad [\hat{c}_n, \hat{H}_0]_+ = \epsilon_n \hat{c}_n$$

$$\hat{c}_n(t) = e^{i\hat{H}_0 t} \hat{c}_n e^{-i\hat{H}_0 t}$$

$$i \frac{\partial}{\partial t} \hat{c}_n(t) = e^{i\hat{H}_0 t} [\hat{c}_n, H_0]_+ e^{-i\hat{H}_0 t} = \epsilon_n \hat{c}_n(t) \quad \longrightarrow \quad \hat{c}_n(t) = e^{-i\epsilon_n t} \hat{c}_n$$

The field operator:

$$\hat{\Psi}(x, t) = \sum_n \hat{c}_n(t) \phi_n(x) = \sum_n e^{-i\epsilon_n t} \phi_n(x) \hat{c}_n$$

Green function for non-interacting systems

The field operator:

$$\hat{\psi}(x, t) = \sum_n \hat{c}_n(t) \phi_n(x) = \sum_n e^{-i\epsilon_n t} \phi_n(x) \hat{c}_n$$

$$\hat{\psi}^\dagger(x') = \sum_n \phi_n^*(x') \hat{c}_n^\dagger$$

The non-interacting Green function:

$$\begin{aligned} G(x, x'; t) &= -i \langle \Phi_0 | T \hat{\psi}(x, t) \hat{\psi}^\dagger | \Phi_0 \rangle \\ &= -i \sum_{nn'} \phi_n(x) \phi_{n'}(x') e^{-i\epsilon_n t} [\theta(t) \langle \Phi_0 | \hat{c}_n \hat{c}_{n'}^\dagger | \Phi_0 \rangle - \theta(-t) \langle \Phi_0 | \hat{c}_{n'}^\dagger \hat{c}_n | \Phi_0 \rangle] \\ &= -i \sum_n \phi_n(x) \phi_n(x') e^{-i\epsilon_n t} [\theta(t) \theta(\epsilon_n - \epsilon_F) - \theta(-t) \theta(\epsilon_F - \epsilon_n)] \end{aligned}$$

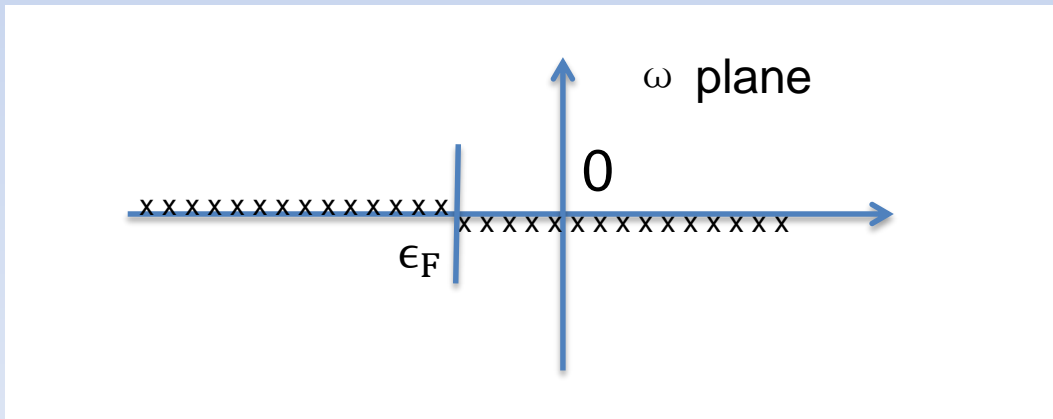
Green function for non-interacting systems

The non-interacting Green function:

$$G(x, x'; t) = -i \sum_n \phi_n(x) \phi_n(x') e^{-i\epsilon_n t} [\theta(t) \theta(\epsilon_n - \epsilon_F) - \theta(-t) \theta(\epsilon_F - \epsilon_n)]$$

Fourier transform to the frequency domain:

$$G(x, x'; \omega) = \int_{-\infty}^{\infty} dt G(x, x'; t) e^{i\omega t}$$
$$= \sum_n \phi_n(x) \phi_n^*(x') \left[\frac{\theta(\epsilon_n - \epsilon_F)}{\omega + i\eta - \epsilon_n} + \frac{\theta(\epsilon_F - \epsilon_n)}{\omega - i\eta - \epsilon_n} \right]$$



Comparison to the interacting cases

The non-interacting Green function:

$$G(x, x'; \omega) = \sum_n \phi_n(x) \phi_n^*(x') \left[\frac{\theta(\epsilon_n - \epsilon_F)}{\omega + i\eta - \epsilon_n} + \frac{\theta(\epsilon_F - \epsilon_n)}{\omega - i\eta - \epsilon_n} \right]$$

This can be compared to the Lehmann representation in the general case:

$$G(x, x'; \omega) = \sum_s \frac{\langle \Psi_0^N | \hat{\Psi}(x) | \Psi_s^{N+1} \rangle \langle \Psi_s^{N+1} | \hat{\Psi}^\dagger(x') | \Psi_0^N \rangle}{\omega - (E_s^{N+1} - E_0^N) + i\eta} +$$

$$\sum_r \frac{\langle \Psi_0^N | \hat{\Psi}(x) | \Psi_r^{N-1} \rangle \langle \Psi_r^{N-1} | \hat{\Psi}^\dagger(x') | \Psi_0^N \rangle}{\omega - (E_0^N - E_r^{N-1}) - i\eta}$$

$$\epsilon_s = E_s^{N+1} - E_0^N = \epsilon_s(N+1) + \mu^+; \quad \mu^+ = E_0^{N+1} - E_0^N, \quad \epsilon_s(N+1) = E_s^{N+1} - E_0^{N+1}$$

$$\epsilon_r = E_0^N - E_r^{N-1} = -\epsilon_r(N-1) + \mu^-; \quad \mu^- = E_0^N - E_0^{N-1}, \quad \epsilon_r(N-1) = E_r^{N-1} - E_0^{N-1}$$

$\mu^+ = \mu^-$: metal; $\mu^+ > \mu^-$: insulator

Classical books

- Abrikosov, Gor'kov, Dzyaloshinskii, *“Quantum field theoretical methods in statistical physics”* (1961, 1963)
- A. Fetter & J. D. Walecka, *“Quantum Theory of Many-particle systems”* (1971)
- G. Mahan, *“Many-particle physics”* (1983) (3rd edition, 2000)