

561 Fall 2005 Lecture 6a

Supplement to Lecture 6: Green's Functions in Many Body Perturbation Theory: T= 0 Formalism

Here we summarize properties of the different Green's functions following Mahan Ch. 2; Other good discussions in Fetter Ch. 3, Abrikosov, et. al., ...

1. The six Green's functions (Copied almost verbatim from Mahan.)

It is convenient to introduce 6 functions. The set of functions provides insight and - more important they are essential for non-equilibrium theories. These are built upon the "time-loop" formalism of Schwinger and were developed by Keldysh for condensed matter applications.

Following Mahan, sec. 2.9, the 6 functions are: retarded, G_{ret} , advanced, G_{adv} , time-ordered, G_t , anti- time-ordered, $G_{\bar{t}}$, and $G^>$ and $G^<$ (no standard names; however, they are related to the Lehman representation as discussed below). Let $x_1 = \mathbf{r}_1, t_1$, etc. Then the functions are:

$$\begin{aligned}
 G^>(x_1, x_2) &= -i\langle\hat{\psi}(x_1)\hat{\psi}^\dagger(x_2)\rangle \\
 G^<(x_1, x_2) &= +i\langle\hat{\psi}^\dagger(x_2)\hat{\psi}(x_1)\rangle \\
 G_t(x_1, x_2) &= \Theta(t_1 - t_2)G^>(x_1, x_2) + \Theta(t_2 - t_1)G^<(x_1, x_2) \\
 G_{\bar{t}}(x_1, x_2) &= \Theta(t_2 - t_1)G^>(x_1, x_2) + \Theta(t_1 - t_2)G^<(x_1, x_2) \\
 G_{ret}(x_1, x_2) &= G_t(x_1, x_2) - G^<(x_1, x_2) \\
 G_{adv}(x_1, x_2) &= G_{\bar{t}}(x_1, x_2) - G^>(x_1, x_2)
 \end{aligned} \tag{1}$$

The functions $G(\mathbf{k}, E)$ are defined by the Fourier transforms. See below.

1a. Expressions for non-interacting hamiltonians

For a noninteracting hamiltonian, the eigenstates are single-body functions $\phi_\lambda(\mathbf{r})$ and the field operators can be written in terms of the creation and annihilation operators:

$$\begin{aligned}
 \hat{\psi}(x_1) &= \sum_\lambda c_\lambda \phi_\lambda(\mathbf{r}_1) e^{-i\epsilon_\lambda t_1} \\
 \hat{\psi}^\dagger(x_1) &= \sum_\lambda c_\lambda^\dagger \phi_\lambda^*(\mathbf{r}_1) e^{i\epsilon_\lambda t_1}
 \end{aligned} \tag{2}$$

The Green's functions for non-interacting electrons are given on the next page.

Green's functions for non-interacting electrons

It is convenient to use occupation numbers for non-interacting electrons, so that the formulas apply to non-zero-temperature, using $n_\lambda = \langle c_\lambda \rangle$, which is the Fermi factor for non-interacting electrons in equilibrium. The Green's functions can be expressed as functions of $t = t_1 - t_2$:

$$\begin{aligned}
 G^>(x_1, x_2) &= -i \sum_{\lambda} (1 - n_{\lambda}) \phi_{\lambda}(\mathbf{r}_1) \phi_{\lambda}^*(\mathbf{r}_2) e^{-i\epsilon_{\lambda} t} \\
 G^<(x_1, x_2) &= +i \sum_{\lambda} n_{\lambda} \phi_{\lambda}(\mathbf{r}_1) \phi_{\lambda}^*(\mathbf{r}_2) e^{-i\epsilon_{\lambda} t} \\
 G_t(x_1, x_2) &= -i \sum_{\lambda} (\Theta(t) - n_{\lambda}) \phi_{\lambda}(\mathbf{r}_1) \phi_{\lambda}^*(\mathbf{r}_2) e^{-i\epsilon_{\lambda} t} \\
 G_{\bar{t}}(x_1, x_2) &= -i \sum_{\lambda} (\Theta(-t) - n_{\lambda}) \phi_{\lambda}(\mathbf{r}_1) \phi_{\lambda}^*(\mathbf{r}_2) e^{-i\epsilon_{\lambda} t} \\
 G_{ret}(x_1, x_2) &= -i \Theta(t) \sum_{\lambda} \phi_{\lambda}(\mathbf{r}_1) \phi_{\lambda}^*(\mathbf{r}_2) e^{-i\epsilon_{\lambda} t} \\
 G_{adv}(x_1, x_2) &= +i \Theta(-t) \sum_{\lambda} \phi_{\lambda}(\mathbf{r}_1) \phi_{\lambda}^*(\mathbf{r}_2) e^{-i\epsilon_{\lambda} t} \tag{3}
 \end{aligned}$$

For the homogeneous gas the states are plane waves and the above equations simplify to:

$$\begin{aligned}
 G^>(\mathbf{k}, t) &= -i(1 - n_{\mathbf{k}}) e^{-i\epsilon_{\mathbf{k}} t} \\
 G^<(\mathbf{k}, t) &= +i n_{\mathbf{k}} e^{-i\epsilon_{\mathbf{k}} t} \\
 G_t(\mathbf{k}, t) &= -i(\Theta(t) - n_{\mathbf{k}}) e^{-i\epsilon_{\mathbf{k}} t} \\
 G_{\bar{t}}(\mathbf{k}, t) &= -i(\Theta(-t) - n_{\mathbf{k}}) e^{-i\epsilon_{\mathbf{k}} t} \\
 G_{ret}(\mathbf{k}, t) &= -i \Theta(t) e^{-i\epsilon_{\mathbf{k}} t} \\
 G_{adv}(\mathbf{k}, t) &= +i \Theta(-t) e^{-i\epsilon_{\mathbf{k}} t} \tag{4}
 \end{aligned}$$

Expressions as a function of energy

Fourier transforming, we find:

$$\begin{aligned}
 G^>(\mathbf{k}, E) &= -2\pi i (1 - n_{\mathbf{k}}) \delta(E - \epsilon_{\mathbf{k}}) \\
 G^<(\mathbf{k}, E) &= +2\pi i n_{\mathbf{k}} \delta(E - \epsilon_{\mathbf{k}}) \\
 G_{ret}(\mathbf{k}, E) &= \frac{1}{E - \epsilon_{\mathbf{k}} + i\eta} \\
 G_{adv}(\mathbf{k}, E) &= \frac{1}{E - \epsilon_{\mathbf{k}} - i\eta} \\
 G_t(\mathbf{k}, E) &= G_{ret} + G^< = \frac{1}{E - \epsilon_{\mathbf{k}} + i\eta_{\mathbf{k}}} \\
 G_{\bar{t}}(\mathbf{k}, E) &= G^< - G_{adv} = \frac{1}{E - \epsilon_{\mathbf{k}} - i\eta_{\mathbf{k}}}, \tag{5}
 \end{aligned}$$

where $\eta > 0$ is a positive infinitesimal whereas $\eta_{\mathbf{k}} > 0$ for $k > k_F$ and $\eta_{\mathbf{k}} < 0$ for $k < k_F$, which changes sign for occupied and empty states. (Note that the order has been changed in this set of equations since G_{ret} and G_{adv} are simple to transform, and one then easily derives G_t and $G_{\bar{t}}$.)

Note that the expression for G_t is the same as we have given before in Lecture 6. Note that the retarded and advanced functions are independent of the occupation; this leads to the simple relation of G_{ret} and G_{adv} to the density of single-body states (see below) independent of whether or not they are occupied. On the other hand, the time-ordered form changes character for occupied and empty states and it is the useful function for perturbation theory in the interaction in a system of electrons.

The last equations are easily generalized to the case of any eigenstates of a non-interacting hamiltonian, using the above definitions. Here we give only the retarded and time-ordered forms:

$$\begin{aligned} G_t(\mathbf{r}_1, \mathbf{r}_2, E) &= \sum_{\lambda} \frac{\phi_{\lambda}(\mathbf{r}_1)\phi_{\lambda}^*(\mathbf{r}_2)}{E - \epsilon_{\lambda} + i\eta_{\lambda}} \\ G_{ret}(\mathbf{r}_1, \mathbf{r}_2, E) &= \sum_{\lambda} \frac{\phi_{\lambda}(\mathbf{r}_1)\phi_{\lambda}^*(\mathbf{r}_2)}{E - \epsilon_{\lambda} + i\eta}, \end{aligned} \quad (6)$$

where $\eta > 0$ is a positive infinitesimal, and $\eta_{\lambda} > 0$ for $\epsilon_{\lambda} > E_F$ and $\eta_{\lambda} < 0$ for $\epsilon_{\lambda} < E_F$.

These expressions are the explicit expressions needed for electron Green's functions: In the perturbation expansions in terms of the interaction, the time-ordered expressions are exactly the functions used in the evaluation of diagrams. Note that one can transform from one type of Green's function to another simply by the placement of the poles in the upper or lower half planes!

1b. Analytic properties for interacting hamiltonians

The important point is that the definition of the six functions applies in general and the analytic properties of the exact functions have the same structure as in the non-interacting case with poles in the same half-planes of the complex plane as for the non-interacting examples.

1c. The density of states and the Lehman Representation

The Lehman or spectral representation was defined in Lecture 5a. The main point is that it represents the spectrum (weighted by matrix elements). For the case of non-interacting Fermions the representation is simply the density of independent-particle states. In terms of the Green's functions, this is a sum of the $G^<$ and $G^>$ forms (with \pm signs for boson and Fermions) and it is simply related to the retarded function:

$$\begin{aligned} \rho(\mathbf{r}_1, \mathbf{r}_2, E) &= -\frac{1}{\pi} \text{Im} G_{ret}(\mathbf{r}_1, \mathbf{r}_2, E) = -\frac{1}{\pi} \text{Im} \sum_{\lambda} \frac{\phi_{\lambda}(\mathbf{r}_1)\phi_{\lambda}^*(\mathbf{r}_2)}{E - \epsilon_{\lambda} + i\eta} \\ \rho(E) &= \int d\mathbf{r} \rho(\mathbf{r}, \mathbf{r}, E) = -\frac{1}{\pi} \sum_{\lambda} \text{Im} \frac{1}{E - \epsilon_{\lambda} + i\eta}. \end{aligned} \quad (7)$$

If the density is resolved into the eigenstates the expressions have the simple form

$$\rho_{\lambda}(E) = -\frac{1}{\pi} \text{Im} G_{ret, \lambda}(E) = -\frac{1}{\pi} \text{Im} \frac{1}{E - \epsilon_{\lambda} + i\eta}. \quad (8)$$

The general relations carry over to the interacting case, except the final equalities in these expressions hold only for non-interacting systems.

2. Analytic properties of the self energy

The proper self energy has been defined by the Dyson equation,

$$G_\lambda(E) = \frac{1}{E - \epsilon_\lambda^0 - \Sigma_\lambda^*(E)}, \quad (9)$$

which is equivalent to

$$G_\lambda(E) = \frac{1}{G_0^{-1}(E) - \Sigma_\lambda^*(E)}. \quad (10)$$

It follows that

$$\Sigma_\lambda^*(E) = G_0^{-1}(E) - G_\lambda^{-1}(E), \quad (11)$$

and it is clear that Σ^* also has the same properties as the Green's functions, with retarded, time-ordered, etc., forms.

3. Phonon Green's functions

Can be derived by the same methods. Done later.