561 Fall 2005 Lecture 6

Green's Functions in Many Body Perturbation Theory: T= 0 Formalism

Following Mahan Ch. 2; Other good discussions in Fetter Ch. 3, Abrikosov, et.el., ... Phillips uses Green's functions in Chapter 6; the example considered there (the impurity Anderson model) will be one of our most instructive examples.

1. Interaction Representation (repeated from before)

(Note distinction from Schrodinger and Heisenberg representations)

Let $H = H_0 + V$, where in general H_0 and V do not commute. Then we define operators in the interaction representation by (Mahan Ch. 2):

$$
\begin{aligned}
\widehat{O}(t) &= e^{iH_0 t} O e^{-iH_0 t} \\
\hat{\psi}(t) &= e^{iH_0 t} e^{-iHt} \hat{\psi}(0) \\
\frac{d\hat{\psi}(t)}{dt} &= -i\widehat{V}(t)\hat{\psi}(t)
\end{aligned}
\tag{1}
$$

If we define $U(t) = e^{iH_0 t} e^{-iHt}$, then $U(0) = 1$, and $\frac{dU(t}{dt} = -i\widehat{V}(t)U(t)$.

Iterative solution:

$$
U(t) = 1 + (-i)\int_0^t dt_1 \widehat{V}(t_1) + (-i)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \widehat{V}(t_1)\widehat{V}(t_2) + \dots
\tag{2}
$$

2. Time ordering operator T

This may be written in a compact form if we define the time ordering operator T which orders operators with earliest times to the right (with a sign change if needed for Fermions):

$T[A(t_i)B(t_j)] = A(t_i)B(t_j)$, if $t_i > t_j$; $= \pm B(t_j)A(t_i)$, if $t_j > t_i$.

[Note the sign change if A and B each have an odd number of Fermion operators. When the operators are interchanged one must change sign to preserve the antisymmetry. However, this is not important at the present step since $\widehat{V}$ always contains only even numbers of Fermion operators.]

Then one can show (see homework)

$$
\begin{aligned}
U(t) &= T[1 + (-i)\int_0^t dt_1 \widehat{V}(t_1) + (-i)^2 \frac{1}{2!} \int_0^t dt_1 \int_0^t dt_2 \widehat{V}(t_1)\widehat{V}(t_2) + (-i)^3 \frac{1}{3!} \dots + \dots \\
&= T\exp(-i\int_0^t dt_1 \widehat{V}(t_1))
\end{aligned}
\tag{3}
$$

3. S matrix

(more complete discussion in Fetter, p. 59-64)

Generalizing the U operator, let $\hat{\psi}(t_1) = S(t_1, t_2)\hat{\psi}(t_2)$.

Then

$$
S(t_1, t_2) = U(t_1)U^+(t_2) = T\exp(-i\int_{t_2}^{t_1} dt_3 \widehat{V}(t_3))
\tag{4}
$$

Key point: We assume that the true solution can be found by starting with the (in principle known) eigenfunctions ϕ_0 of the non-interacting Hamiltonian H_0 and "turning on" V "adiabatically". That is, in the distant past, the solutions were ϕ_0 and the true solutions

at the present can be derived from ϕ_0 by applying the S operator: $\hat{\psi}(t) = S(t, -\infty)\hat{\psi}(-\infty) = S(t, -\infty)\phi_0(-\infty) = S(t, -\infty)\phi_0(0)$ This is discussed in Fetter, p. 59-64, where "turning on" is explicitly discussed with a hamiltonian $H = H_0 + e^{-\epsilon|t|}V$, with ϵ a small positive infinitesimal. It is shown that the expressions for $\hat{\psi}(t) = S(t, -\infty)\phi_0(0)$ do not have a well-defined limit as $\epsilon \to 0$; nevertheless the Gellmann-Low theorem shows that the objects we actually use are well-defined. Later we will see that as a consequence, one can construct Green's functions in the form of ratios where both numerator or denominator diverge, but their ratio is a meaningful subset of all the possible terms in the expansion for the numerator.

The assumption that the true states are correctly derived by starting from H_0 and "turning on" V is the basic assumption of Fermi Liquid Theory. More generally, it is the assumption that no 'phase transition" occurs as V is introduced. For now we will assume that $S(t, -\infty)$ is well-defined and describes the interacting system properly. The latter part of the course deals with cases where there is a transition to a new state of order, e.g., to the superconducting state. Even then the Green's functions are very useful - they diverge where the transitions actually occur. Also we will follow Mahan and use the same type of analysis for large positive times, with the choice that the non-interacting eigenfunctions at $t = \infty$ differ only by a phase factor from those at $t = -\infty$:
$\hat{\psi}(\infty) = S(\infty, -\infty)\phi_0(-\infty) = S(\infty, -\infty)\phi_0(0) = e^{iL}\phi_0(0)$
(Once again, Fetter gives a more rigorous discussion.)

4. Time-ordered Green's Functions
See, e.g., Mahan, section 2.3.
Define the Green's function by

$$G_{AB}(t_1 - t_2) = -i\langle T[A^H(t_1)B^H(t_2)]\rangle, \tag{5}$$

where $O^H(t)$ denotes a Heisenberg operator - (Note: the operators are in the Heisenberg representation – NOT the interaction representation). This is similar to the form we defined earlier for the retarded G. [In fact all the different G's differ only in the way the terms for $t_1 > t_2$ and $t_1 < t_2$ are treated.] In a homework exercise you are asked to show that this G also is an appropriate Green's function.

Examples for non-interacting cases:
A. fermions (electrons) in the vacuum where $|0\rangle$ is the empty state:

$$\begin{aligned}
G_k^0(t_1 - t_2) &= -i\langle 0|T[c(t_1)c^+(t_2)]|0\rangle \\
&= -i\Theta(t_1 - t_2)\langle 0|c(t_1)c^+(t_2)|0\rangle \\
&= -i\Theta(t_1 - t_2)e^{-i\epsilon_k(t_1 - t_2)}
\end{aligned} \tag{6}$$

Fourier transform:

$$G_k^0(E) = \frac{1}{E - (\epsilon_k - i\delta)}, \tag{7}$$

where $\delta > 0$ is the convergence factor so the integral is well defined at large positive time $t = t_1 - t_2$. Thus $G_k^0(E)$ has a pole in the lower half plane with $ImE < 0$.
B. Degenerate Gas with $|0\rangle$ the filled Fermi sea.
Now there are contributions from both time orderings and the result is:

$$G_k^0(E) = \frac{\Theta(\epsilon_k - \mu)}{E - (\epsilon_k - i\delta)} + \frac{\Theta(\mu - \epsilon_k)}{E - (\epsilon_k + i\delta)}, \tag{8}$$
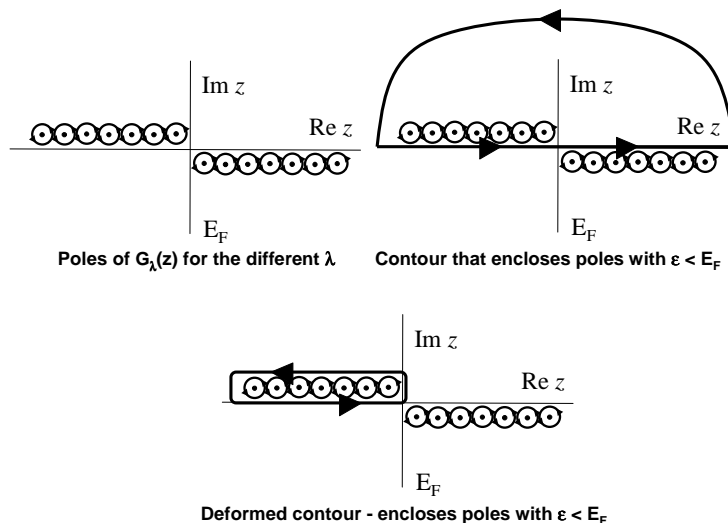
Figure 1: Poles for the one-electron Green's function.

where μ is the Fermi energy. Note that the poles are in the lower plane for $\epsilon_k > \mu$ and in the upper plane for $\epsilon_k < \mu$.

C. Phonons. See notes and Mahan

Interacting cases:

This Heisenberg form is in general *not* possible to use *directly* since we usually do not know the eigenstates of H nor is the Heisenberg form for the operators something we can deal with for general Hamiltonians. However, we can work with a non-interacting H_0 and we can find an *iterative solution* for $H = H_0 + V$. As Mahan shows, the result can be written

$$G_{AB}(t_1 - t_2) = -i \frac{{}_0\langle T[A^H(t_1)B^H(t_2)]S(\infty, -\infty)\rangle_0}{{}_0\langle S(\infty, -\infty)\rangle_0}, \tag{9}$$

where the subscript 0 means expectation with ϕ_0, the ground state of H_0.

This compact form is really just shorthand for the expression which can be derived by combining this expression with the above definition for any time-ordered matrix element to give the expression: (Mahan 2.4.1)

$$G_{AB}(t_1 - t_2) = -i \sum_{n=0} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_3 \int_{-\infty}^{\infty} dt_4 \ldots \frac{{}_0\langle T[A^H(t_1)B^H(t_2)\widehat{V}(t_3)\widehat{V}(t_4)\ldots]\rangle_0}{{}_0\langle S(\infty, -\infty)\rangle_0}. \tag{10}$$

(We will see that one does not need to treat directly the denominator.) Since $\widehat{V}(t) = e^{iH_0 t}V(t)e^{-iH_0 t}$, each term in this expansion involves only the unperturbed H_0, and one can develop a set of rules to evaluate the expressions at any order.

5. Wick's Theorem

The utility of Wick's theorem is that it greatly simplifies evaluation of any of the terms in the expansion of the Green's function. The key point is that each term in the expansion

is involves only the unperturbed Hamiltonian H_0 and its eigenstates. Therefore a straight-forward set of rules can be given. Wick's theorem states that each time-ordered matrix element of n creation and n destruction operators can be written as a sum of n! terms, each a product of n paired matrix elements of the form $\langle T[c(t_1)c^+(t_2)]\rangle$ for Fermions and similar terms for bosons. These are simply evaluated as the Green's functions G_0 for the Hamiltonian H_0. The sign conventions are that for Fermions we must change sign each time operators are exchanged to get to the form with the creation operator to the right (the convention in G_0).

For equal times, the Green's functions are defined by the usual rules for expectation values for the given operators, e.g., for non-interacting fermions, $\langle c_{k_1}c_{k_2}^+\rangle = \delta_{k_1,k_2}n(\epsilon_{k_1} - \mu)$

6. Feynman Graphs
Graphical representation of the diagrams that result from Wick's decomposition.
Note that the exact rules for Feynman Graphs depend upon the problem.
7. Linked Graphs: Elimination of Disconnected Graphs - (Vacuum Polarization Graphs)
A great simplification is that we sum over only linked (connected) distinct graphs. It turn out (See Mahan sec. 2.9 and more complete proofs in Fetter.) that this corresponds exactly to cancelling the factor of $_0\langle S(\infty, -\infty)\rangle_0$ in the denominator. In addition each connected graphs has n! permutations which are all equivalent, so that if we consider only distinct, connected graphs, the factor of n! can be cancelled and one finds

$$G_{AB}(t_1-t_2) = -i \sum_{n=0}(-i)^n \int_{-\infty}^{\infty} dt_3 \int_{-\infty}^{\infty} dt_4 \ldots {}_0 \langle T[A^H(t_1)B^H(t_2)\widehat{V}(t_3)\widehat{V}(t_4)\ldots]\rangle_{0 distinct,connected} (11)$$

Explicit rules for Feynman graphs, with all signs and imaginary factors are given in Mahan, Sect. 2.8. See also other texts like Fetter.

8. Frequency or energy representation
The simplest expressions are for the Fourier transform:

$$G(E) = \int_{-\infty}^{\infty} dt e^{iEt} G(t). \tag{12}$$

The unperturbed G's have the simple forms given above, such as:

$$G_\lambda^0(E) = \frac{1}{E - \epsilon_\lambda^0 \pm i\delta}, \tag{13}$$

where δ is a positive infinitesimal (see above).

Examples of the analytic structure for independent particles: For fermions at $T = 0$ the poles are in the lower plane for $E > \mu$ and in the upper plane for $E < \mu$. Similarly for phonons, at $T = 0$ the poles are in the lower plane for $E > 0$ and in the upper plane for $E < 0$. Thus these functions do *not* obey the relations for causal functions, such as the Kramers-Kronig relations.

The expansion of G can be given in powers of the G^0's. Each product of G^0's involves integrals over energy for each G^0, and one integral can be done immediately using conservation of energy.) However, this is not the most useful approach. See below.

9. Dyson's Equation and (Proper) Self Energies $\Sigma^\star$

This is perhaps the *most useful equation in all the Green's function analysis* **in terms of understanding the** *meaning* **of the Green's functions and response functions in condensed matter. The analysis holds for all types of Green's functions, not just time-ordered functions; for example, this is the most convenient form for response functions such as the dielectric function as shown in the previous lecture.**

The key result is that the exact Green's function equation can *always* be written as the Dyson equation:

$$G_\lambda(E) = G_\lambda^0(E) + G_\lambda^0(E)\Sigma(E)_\lambda G_\lambda^0(E) \equiv G_\lambda^0(E) + G_\lambda^0(E)\Sigma_\lambda^\star(E)G_\lambda(E), \tag{14}$$

See schematic figure for Dyson Equation.

Here $\Sigma_\lambda^\star(E)$ is the proper self-energy. The subscript λ denotes the quantum numbers that are assumed to be conserved in the full interacting problem, e.g., momentum and fermion statistics. (Mahan defines only the latter proper self-energy and he omits the designation "proper". I think it is much better to define $\Sigma^\star$ as in Fetter.) The distinction is that $\Sigma^\star$ is the simpler "irreducible" set of diagrams that cannot be cut by cutting a single G^0 line, whereas $\Sigma(E)$ is an infinite series of terms like $\Sigma^\star$. Thus $\Sigma^\star$ is always the simpler object to be preferred in calculations and in interpretation.

Using the simple expression above for G^0, it is easy to show that G can *always* be written as

$$G_\lambda(E) = \frac{1}{E - \epsilon_\lambda^0 - \Sigma_\lambda^\star(E)}, \tag{15}$$

where $\Sigma_\lambda^\star(E)$ is defined for complex values of the energy E. Thus $Im\Sigma_\lambda^\star(E)$ must be defined properly so that the Green's function has the proper analytic structure for $G^{time-ordered}$, $G^{retarded}$, etc. This means that $\Sigma_\lambda^\star(E)$ also is time-ordered, retarded, etc.

The proper self energy has the interpretation of the modification of the independent particle energy due to the effects of the interactions. This is the must useful quantity for our studies.

10. Quasiparticles and Collective Excitations
The for of the true interacting particle Green's function in terms of the Dyson's equation and the proper self-energy is the key to two of the most important ideas in this course (and in condensed matter theory): Quasiparticles and Collective Excitations

This is the subject of the next lectures.

11. Examples
Hartree Fock: See figure giving diagrams for the H-F self-energy $\Sigma_\lambda^{\star\,HF}(E) = \Sigma_\lambda^{\star\,Hartree} + \Sigma_\lambda^{\star\,Fock}$. More details are given in Fetter, Mahan, Ch. 2,5

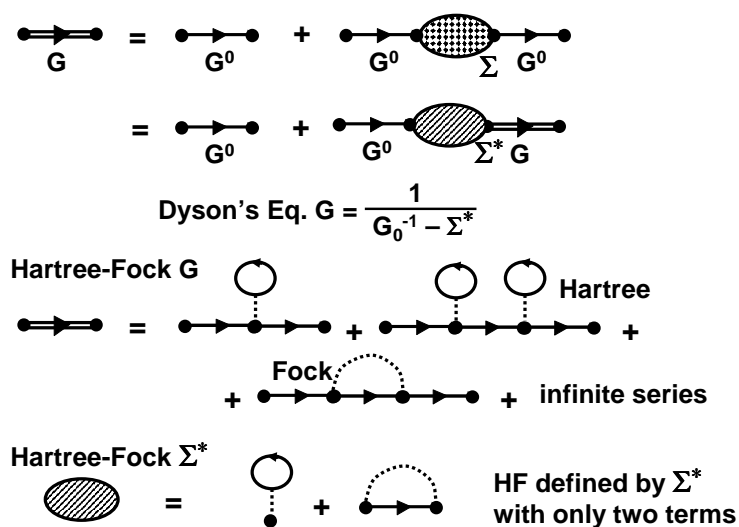Electron-phonon interaction: See Mahan, Ch. 2

Figure 2: One-electron Green's function and self energy. The Dyson Eq. is in terms of the proper self energy $\Sigma^\star_\lambda(E)$ for a state with quantum numbers λ. At the bottom are shown the expressions in the Hartree-Fock approximation.