

### 561 Fall 2005 Lecture 14

#### Green's Functions at Finite Temperature: Matsubara Formalism

Following Mahan Ch. 3

##### 1. Recall from $T=0$ formalism

- In terms of the exact hamiltonian  $H$  the Green's function is given by operators in the Heisenberg representation  $O^H(t) = e^{iHt} O e^{-iHt}$ . The time-ordered form is

$$G_{AB}^T(t_1 - t_2) = -i \langle T[A^H(t_1)B^H(t_2)] \rangle, \quad (1)$$

and the retarded form is

$$G_{AB}^{ret}(t_1 - t_2) = -i \langle [A^H(t_1), B^H(t_2)] \rangle, \quad (2)$$

where  $[,]$  denotes a commutator (boson) or anticommutator (fermion).

- **Interaction Representation**

If  $H = H_0 + V$ , operators in the interaction representation can be written as

$$\hat{O}(t) = e^{iH_0 t} O e^{-iH_0 t} \quad (3)$$

This is useful for expansion in powers of  $V$ .

- Examples for non-interacting electrons

A. Fermions (electrons) in the vacuum where  $|0\rangle$  is the empty state. For either retarded or time-ordered:

$$\begin{aligned} G_k^0(t_1 - t_2) &= -i \langle 0 | T[c(t_1)c^+(t_2)] | 0 \rangle \\ &= -i \Theta(t_1 - t_2) \langle 0 | c(t_1)c^+(t_2) | 0 \rangle \\ &= -i \Theta(t_1 - t_2) e^{-i\epsilon_k(t_1 - t_2)} \end{aligned} \quad (4)$$

Fourier transform:

$$G_k^0(E) = \frac{1}{E - (\epsilon_k - i\delta)}, \quad (5)$$

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.

For time-ordered case, there are contributions from both time orderings and the result is:

$$G_k^0(E) = \frac{\Theta(\epsilon_k - \mu)}{E - (\epsilon_k - i\delta)} + \frac{\Theta(\mu - \epsilon_k)}{E - (\epsilon_k + i\delta)}, \quad (6)$$

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

- The time ordered function is the one that is most convenient for calculations because it is needed in the expansions in terms of the interactions.
- For interacting electrons (Mahan ch. 2): Green's function expansion  $\rightarrow$  Dyson's Eq. and proper self energies  $\Sigma^*$  derived for time-ordered G.
- The retarded function is the same except the pole for  $\epsilon_k < \mu$  is shifted to the lower plane. The retarded functions are needed for relation to experimental measurements.
- To find retarded G in interacting case, first do time ordered, then convert to retarded.

## 2. Finite temperature - One possible form

The above expressions are valid also for  $T \neq 0$  where  $\langle \rangle$  means thermal expectation value in the grand canonical ensemble, so that

$$G_{AB}^T(\beta, t_1 - t_2) = -iTr \left[ e^{-\beta(\hat{H} - \mu\hat{N} - \Omega)} T[A^H(t_1)B^H(t_2)] \right]. \quad (7)$$

where  $\beta = 1/kT$ . The electron Greens functions is

$$G_p^T(\beta, t_1 - t_2) = -iTr \left[ e^{-\beta(\hat{H} - \mu\hat{N} - \Omega)} T[e^{i\hat{H}t_1} c_p e^{i\hat{H}(t_2 - t_1)} c_p^\dagger e^{-i\hat{H}t_2}] \right], \quad (8)$$

where

$$e^{-\beta\Omega} = Tr \left[ e^{-\beta(\hat{H} - \mu\hat{N})} \right]. \quad (9)$$

If we work (formally) in the basis of the exact states  $|n\rangle$ , and Fourier transform, this leads to the expression for the retarded function

$$G_{ret}(p, \omega) = e^{\beta\Omega} \sum_{n,m} |\langle n|c_p|m\rangle|^2 \frac{e^{-\beta E_n} + e^{-\beta E_m}}{\omega + E_n - E_m + i\delta}, \quad (10)$$

and similar expressions for other functions.

Free particle expressions have thermal factors as we have described before.

## 3. Finite Temperature and complex time/temperature

There is a problem, however, in practice: if we consider define  $H = H_0 + V$  and express the Green's function as an expansion in  $V$ , then  $V$  appears in both the thermal factor and in the time dependence. There appear to be two types of expansions required.

The solution is to realize that the factors of the form  $e^{-\beta H + iHt}$  can be treated together in terms of a complex time in which  $t$  and  $\beta$  are the real and imaginary parts.

### Intermediate Step: Free fermion and boson occupation functions in the complex plane

The well-known occupation functions

$$n(z) = \frac{1}{e^{\beta z} \pm 1} \quad (11)$$

are *periodic functions* for  $z$  along the imaginary axis ( $z = iy$  where  $y$  is real) with poles at  $z = i\omega_n$ , where  $\omega_n = \frac{\pi}{\beta} 2n$  for bosons,  $\omega_n = \frac{\pi}{\beta} (2n + 1)$  for fermions.

The value at any  $z$  can be determined from the residues of the poles:

$$n(z) = \frac{1}{e^{\beta z} \pm 1} = \pm \frac{1}{2} + \frac{1}{\beta} \sum_n \frac{1}{i\omega_n - z} \quad (12)$$

### 5. Matsubara form

The key to the Matsubara form is to define Green's functions for imaginary time  $\tau = it$  which is like inverse temperature  $\beta$ . Then one can use all the algebra of the time ordered formalism (Feynman linked diagrams, Wick's theorem, ...). The expressions are even easier than at  $T=0$  because the frequency sum can be done more easily. In addition by simple analytic continuation one gets directly the retarded Green's function in real frequencies.

The Matsubara form treats time as a complex temperature. If we define  $\tau = it$ , and  $\hat{K} = \hat{H} - \mu\hat{N}$  for the grand canonical ensemble, then the  $\tau$ -ordered Greens function by

$$\begin{aligned} \mathcal{G}_k(\tau_1 - \tau_2) &= -\langle T_\tau c_p(\tau_1) c_p^\dagger(\tau_2) \rangle \\ &= -Tr \left[ e^{-\beta(\hat{K}-\Omega)} T_\tau [e^{\tau_1 \hat{K}} c_k e^{(\tau_2 - \tau_1) \hat{K}} c_k^\dagger e^{-\tau_2 \hat{K}}] \right] \end{aligned} \quad (13)$$

where

$$c_p(\tau) = e^{\tau \hat{K}} c_p e^{-\tau \hat{K}}. \quad (14)$$

(Here we explicitly indicate that  $\hat{K}$  is an operator whereas  $\Omega$  is a number.) It is straightforward to show  $\mathcal{G}$  is a function of  $\tau = \tau_1 - \tau_2$  by cyclic permutation of operators in  $Tr$ .

### (Anti)periodicity as a function of $\tau$ and Fourier transform

- Periodic or antiperiodic for  $\tau \rightarrow \tau + \beta$ . Proof (given in Mahan, Ch. 3, and many other texts) uses cyclic permutation of operators. Consider  $\tau > 0$ :

$$\mathcal{G}_k(\tau) = e^{\beta\Omega} Tr \left[ e^{-\beta\hat{K}} e^{\tau\hat{K}} c_k e^{-\tau\hat{K}} c_k^\dagger \right] = e^{\beta\Omega} Tr \left[ e^{(\tau-\beta)\hat{K}} c_k e^{-\tau\hat{K}} c_k^\dagger \right] \quad (15)$$

If we let  $\tau' = \tau - \beta$  and permute the operators in the above expression, we find

$$\mathcal{G}_k(\tau) = e^{\beta\Omega} Tr \left[ e^{\tau'\hat{K}} c_k e^{-(\tau+\beta)\hat{K}} c_k^\dagger \right] = e^{\beta\Omega} Tr \left[ e^{-\beta\hat{K}} e^{\tau'\hat{K}} c_k^\dagger e^{-\tau'\hat{K}} c_k \right] \quad (16)$$

or

$$\mathcal{G}_k(\tau) = -\mathcal{G}_k(\tau') = -\mathcal{G}_k(\tau - \beta). \quad (17)$$

Thus for fermions  $\mathcal{G}_k(\tau) = -\mathcal{G}_k(\tau - \beta)$  and the entire function is determined by the values on the interval  $0 < \tau < \beta$ . (For bosons the proofs are identical except  $\mathcal{D}_k(\tau) = +\mathcal{D}_k(\tau - \beta)$ .)

- Since  $\mathcal{G}$  is periodic with period  $2\beta$ , it is determined by a discrete set of Fourier components. Using the antiperiodic character derived above, the Fourier Transform is given by the integral over the finite interval

$$\mathcal{G}(k, i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \mathcal{G}_k(\tau), \quad (18)$$

where  $\omega_n = (2n+1)\frac{\pi}{\beta}$  for fermions. (For bosons,  $\mathcal{D}$  is periodic with period  $\beta$  and the Fourier components are for frequencies  $\omega_n = (2n)\frac{\pi}{\beta}$ .)

- Free fermions:

$$\mathcal{G}(k, i\omega_n) = \frac{1}{i\omega_n - \epsilon_k}, \quad (19)$$

which is the same as the expression for real frequency ( $E = \omega$ ) with  $i\omega \rightarrow \omega + i\delta$

- T dependence is completely in the positions of the poles!
- Result: For all Green's functions (free and interacting; boson and fermion) the Matsubara form reduces to the retarded form at real frequency with the analytic continuation  $i\omega \rightarrow \omega + i\delta$ . This is an analytic continuation from the imaginary frequency axis to the real axis.

### 6. Wick's Theorem, diagrams, Dyson's Eq., self energies, etc., work just as for $T = 0$

Sum over all internal momenta (conserving momentum at each vertex) and either: 1) integrate over all internal  $0 < \tau < \beta$ , or 2) sum over all internal  $i\omega_n$  (conserving energy at each vertex)

Exact rules are given in Mahan, Ch. 3 and other texts.

The integrals become sums and are easier in actual calculations!

One difference is that Wick's theorem is an operator identity in the  $T = 0$  formalism; in the Matsubara form the contractions are valid for the thermal expectation values only. Thus the theory is restricted to thermal equilibrium and has not been generalized to non-equilibrium ensembles.

### 7. Advantages of Matsubara formalism

A key advantage is that it is a thermal equilibrium theory. Sometimes the limit of  $T \rightarrow 0$  is not the same as the  $T = 0$  result. Which is right? The  $T \rightarrow 0$  formalism is designed to get the true ground state including an equal thermal occupation of degenerate states. The  $T = 0$  may find only one of the degenerate states or it may find an excited state as a result of the "adiabatic turning on of the interaction" which may not find a crossing of states or a phase transition.

### 8. Example - Green's function for an isolated atom (the Anderson impurity model in the isolated limit)

In the  $T = 0$  formalism we described in words a transition (or crossover) between states with different degeneracies as a function of occupation or Fermi energy. In the finite  $T$  formalism it is natural. The energy of the state as a function of occupation  $n$  is

$$E_n = n\epsilon + \frac{n(n-1)}{2}U, \quad (20)$$

and the partition function is given by

$$Z = \sum_{n=0}^N Z_n e^{-\beta E_n}, \quad (21)$$

where  $Z_n$  is the number of ways  $n$  particles can be placed in  $N$  states,  $Z_n = N!/(n!(N-n)!)$ .

The Green's function is

$$\mathcal{G}(i\omega_m) = - \sum_{\nu} \int_0^{\beta} d\tau e^{i\omega_m \tau} \langle T_{\tau} c_{\nu}(\tau) c_{\nu}^{\dagger} \rangle, \quad (22)$$

and in terms of the energies  $E_n$  for  $n$  electrons, it becomes

$$\mathcal{G}(i\omega_m) = \frac{1}{Z} \sum_{n\nu} Z_n \langle n | c_{\nu} | n+1 \rangle \langle n+1 | c_{\nu}^{\dagger} | n \rangle \frac{e^{-\beta E_n} + e^{-\beta E_{n+1}}}{i\omega_m + E_n - E_{n+1}}. \quad (23)$$

Using the relation  $Z_{n+1} = Z_n \frac{N-n}{n+1}$ , this leads to the form

$$\mathcal{G}(i\omega_m) = \frac{1}{Z} \sum_n Z_n e^{-\beta E_n} \left[ \frac{N-n}{i\omega_m + E_n - E_{n+1}} + \frac{n}{i\omega_m + E_{n-1} - E_n} \right]. \quad (24)$$

This has a very simple interpretation as the thermal weighted average of all possible addition and removal transitions. The retarded Green's function  $G_{ret}(\omega)$  is found by substituting  $i\omega_m \rightarrow \omega + i\eta$ ,  $\eta > 0$ . The delta function peaks in the  $ImG_{ret}(\omega)$  are the addition and subtraction energies of the Anderson impurity model with no hybridization with the surrounding metal.

### 9. Anderson impurity model including hybridization

This is not done here. Good problem for a project. Using the large  $N$  approximation, one can determine the spectra (including the Kondo resonance at the Fermi energy) and the temperature dependence (where the resonance goes away for  $T \gg T_K$ ).

### 10. Finite Temperature Green's Function in the Hartree-Fock Approximation

The equation of motion for the operator  $c_{\mathbf{p},\sigma}(\tau)$  is (Here  $V$  is the volume often omitted in other expressions.)

$$\frac{\partial c_{\mathbf{p},\sigma}(\tau)}{\partial \tau} = [H, c_{\mathbf{p},\sigma}(\tau)] = -\xi_{\mathbf{p}} c_{\mathbf{p},\sigma} - \frac{1}{V} \sum_{\mathbf{p}',\sigma',\mathbf{q} \neq 0} v_{\mathbf{q}} c_{\mathbf{p}'-\mathbf{q},\sigma'}^{\dagger} c_{\mathbf{p}',\sigma'} c_{\mathbf{p}-\mathbf{q},\sigma}$$

Using the definition of the Green's function and the result of part (a), we get that

$$\begin{aligned} \frac{\partial G(\mathbf{p}, \tau)}{\partial \tau} &= -\delta(\tau) - \langle T_{\tau} \left[ \frac{\partial c_{\mathbf{p},\sigma}(\tau)}{\partial \tau} \right] c_{\mathbf{p},\sigma}^{\dagger}(0) \rangle \\ &= -\delta(\tau) - \xi_{\mathbf{p}} G(\mathbf{p}, \tau) + \frac{1}{V} \sum_{\mathbf{p}',\sigma',\mathbf{q} \neq 0} v_{\mathbf{q}} \langle T_{\tau} c_{\mathbf{p}'-\mathbf{q},\sigma'}^{\dagger}(\tau) c_{\mathbf{p}',\sigma'}(\tau) c_{\mathbf{p}-\mathbf{q},\sigma}(\tau) c_{\mathbf{p},\sigma}^{\dagger}(0) \rangle \end{aligned}$$

In the Hartree-Fock approximation

$$\langle T_{\tau} c_{\mathbf{p}'-\mathbf{q},\sigma'}^{\dagger}(\tau) c_{\mathbf{p}',\sigma'}(\tau) c_{\mathbf{p}-\mathbf{q},\sigma}(\tau) c_{\mathbf{p},\sigma}^{\dagger}(0) \rangle \approx n_{\mathbf{p}-\mathbf{q},\sigma} G(\mathbf{p}, \tau)$$

After the Fourier transform we get

$$G(\mathbf{p}, ip_n) = \frac{1}{ip_n - \xi_{\mathbf{p}}} + \frac{1}{V} \sum_{\mathbf{q} \neq 0} v_{\mathbf{q}} n_{\mathbf{p}-\mathbf{q}}$$

The self energy term is

$$\Sigma(\mathbf{p}, ip_n) = -\frac{1}{V} \sum_{\mathbf{q} \neq 0} v_q n_{\mathbf{p}-\mathbf{q}}$$

This term was calculated in homework 4 for zero temperature. Here we note that for non-zero temperature the HF singularity at the Fermi surface is removed..