CHAPTER IV

GREEN'S FUNCTION TECHNIQUE

IV.1 Double Time Temperature Dependent Green's Functions

The double-time retarded and advanced temperature dependent Green's function $\langle\langle A(t); B(t')\rangle\rangle^{\{r \atop a\}}$ are defined as[20]

$$\langle\langle A(t); B(t')\rangle\rangle^{\{r \atop a\}} = \{\mp\} i\theta\left[\{\pm\}(t-t')\right]\langle [A(t), B(t')]_{\pm}\rangle \qquad (4.1)$$

where $\langle \cdots \rangle$ denotes a grand canonical ensemble average,

$$\theta(x) = \begin{cases} 1, & x>0, \\ 0, & x<0, \end{cases}$$ is the Heaviside function

and $[\ \ ]_{\pm}$ denotes an anticommutation or commutation relation.

The operator A(t) and B(t) are general products of quantized field operators or of particle creation and destruction operators in the generalized Heisenberg picture. By generalized Heisenberg picture we mean that

$$A(t) = e^{i\mathcal{H}t} A e^{-i\mathcal{H}t}, \qquad (\hbar = 1)$$

where $\mathcal{H} = H - \mu N$. Here H is the ordinary Hamiltonian operator, μ the chemical potential, and N the total number of particles operator.

From the above definition, we find that both the retarded and advanced Green's function satisfy the following differential equation

$$i\frac{d}{dt}\langle\langle A(t);B(t')\rangle\rangle = \delta(t-t')\langle[A(t),B(t')]_{\pm}\rangle + \langle\langle[A(t),H(t)];B(t')\rangle\rangle . \tag{4.2}$$

Of course, the advanced and retarded Green's functions will satisfy different boundary conditions.

From the definitions of the Green's functions, it follows that they are functions of t-t' only in the case of statistical equilibrium. Hence we introduce the Fourier transforms

$$\langle\langle A;B\rangle\rangle_{\omega}^{\{{r \atop a}\}} = \frac{1}{2\pi}\int_{-\infty}^{\infty}\langle\langle A(t);B(t')\rangle\rangle^{\{{r \atop a}\}} e^{i\omega(t-t')}\, d(t-t'), \tag{4.3}$$

defined for real ω .

Now because of the Heaviside function in the definitions of $\langle\langle A(t);B(t')\rangle\rangle^{\{{r \atop a}\}}$, it follows that $\langle\langle A;B\rangle\rangle_{\omega}^{r}$ can be analytically continued into the entire upper half complex ω plane, and $\langle\langle A;B\rangle\rangle_{\omega}^{a}$ into the entire lower half complex ω plane. We then define the function

$$G_{AB}(\omega) = \langle\langle A;B\rangle\rangle_{\omega} = \begin{cases}\langle\langle A;B\rangle\rangle_{\omega}^{r}, & \text{if } Im\,\omega>0,\\ \langle\langle A;B\rangle\rangle_{\omega}^{a}, & \text{if } Im\,\omega<0,\end{cases} \tag{4.4}$$

assuming ω to be complex.

This is a very convenient definition because $\langle\langle A;B\rangle\rangle_{\omega}$ satisfies the simple equation

$$\omega\langle\langle A;B\rangle\rangle_{\omega} = \frac{1}{2\pi}\langle[A,B]_{\pm}\rangle + \langle\langle[A,H]_{+};B\rangle\rangle_{\omega}, \tag{4.5}$$

which follows from Eq.(4.2) and definition (4.3) and(4.4)

The function $\langle\langle A;B\rangle\rangle_\omega$ is analytic in both the upper and lower halves of the complex ω-plane with poles or discontinuities on the real axis. The spacial case of $A=c_k$ and $B=c^+_{k'}$, where k and k' label states of a complete orthonormal set of one-particle states, gives the so-called "one particle Green's function $\langle\langle c_k;c^+_{k'}\rangle\rangle_\omega$". They are of particular interest since they determine the one-particle time correlation $\langle c^+_{k'}(t)\,c_k(0)\rangle$ which fully describe all one-particle properties of a system in equilibrium. The explicit relation between the correlation function and the one-particle Green's function is

$$\langle B(t')A(t)\rangle = i\lim_{\epsilon\to 0^+}\int_{-\infty}^{\infty}\frac{\left[\langle\langle A;B\rangle\rangle_{\omega+i\epsilon}-\langle\langle A;B\rangle\rangle_{\omega-i\epsilon}\right]e^{-i\omega(t-t')}\,d\omega}{e^{\beta\omega}\pm 1}$$

$$= \int_{-\infty}^{\infty} J_{BA}(\omega)\,e^{-i\omega(t-t')}\,d\omega\,, \qquad (4.6)$$

where $$J_{BA}(\omega) = i\lim_{\epsilon\to 0^+}\frac{\left[\langle\langle A;B\rangle\rangle_{\omega+i\epsilon}-\langle\langle A;B\rangle\rangle_{\omega-i\epsilon}\right]}{e^{\beta\omega}\pm 1}\,, \qquad (4.7)$$

is called the "spectral intensity function" of $\langle B(t')A(t)\rangle$.

For a system of large number of interacting particles, the one-particle Green's function will have a cut along the real axis rather than poles. We expect poles only in a first approximation. The poles can be identified with the energy spectrum of elementary excitations of the system. A cut indicates damping. The time correlation function will oscillate as $|t-t'|\to\infty$ with finite damping.

We also can prove that the Green's functions $\langle\langle c_k ; c^+_{k'} \rangle\rangle_\omega$ determine the ground state energy even when there are two-particle interactions. Therefore, it is usually sufficient to calculate only the one-particle Green's functions to get all the information we want to know about a given system.

The problem in using the double-time temperature dependent Green's function is knowing how to trunicate the hierachy of coupled equations arising from (4.5). Since $\langle\langle [A,H]_+ ; B \rangle\rangle_\omega$ will most likely result in higher order Green's function. Brieftly mention that the hierachy of equations is connected to the diagram technique, i.e., every time we see a line, a bubble or any thing in the diagram representation, we can be sure that there is an equivalent term in the hierachy of coupled equation.

To trunicate the hierachy of equations arising in our study, we have used the Hartree-Fock approximation

$$A^+B^+CD = \langle A^+B^+\rangle CD + \langle CD\rangle A^+B^+ - \langle A^+C\rangle B^+D - \langle B^+D\rangle A^+C, \qquad (4.8)$$

The above approximation is used to treat both the BCS term and the Coulomb repulsion term appearing in the Anderson Hamiltonian in chapter I. The approximation has also been used to treat both terms simultaneously in the study of transition metal impurities in simple superconductors.

IV.2 Self-Consistent Solutions

We want to obtain the Green's functions or propagators for the s-electrons so we must evaluate the commutations of the four operators $c^{+}_{k\sigma}$, $c_{k\sigma}$, $d^{+}_{j\sigma}$ and $d_{j\sigma}$ with the Anderson Hamiltonian(3.9) i.e.,

$$
\begin{aligned}
H = & \sum_{k,\sigma} \epsilon_k c^{+}_{k\sigma} c_{k\sigma} + \sum_{j,\sigma} (E_j + U\langle n_\sigma \rangle) d^{+}_{j\sigma} d_{j\sigma} \\
& + \sum_{j,k,\sigma} (V_{kj} c^{+}_{k\sigma} d_{j\sigma} + V^{*}_{jk} d^{+}_{j\sigma} c_{k\sigma}) \\
& - \frac{1}{2} \sum_{j,\sigma} (\Delta^{*}_{g} d_{j-\sigma} d_{j\sigma} + \Delta_g d^{+}_{j\sigma} d^{+}_{j-\sigma}).
\end{aligned}
$$

Using the relationship

$$[A, BC] = \{A, B\} C - B \{A, C\}, \qquad (4.9)$$

where $[\ \ ]$ denotes the commutation and $\{\ \ \}$, the anticommutation, we obtain

$$[c^{+}_{k\sigma}, H] = -\epsilon_k c^{+}_{k\sigma} - \sum_j V^{*}_{kj} d^{+}_{j\sigma}, \qquad (4.10.a)$$

$$[c_{k\sigma}, H] = \epsilon_k c_{k\sigma} + \sum_j V_{jk} d_{j\sigma}, \qquad (4.10.b)$$

$$[d_{j\sigma}, H] = (E_j + U\langle n_\sigma \rangle) d_{j\sigma} - \Delta_g d^{+}_{j-\sigma} + \sum_{\ell} V^{*}_{\ell j} c_{\ell\sigma}, \qquad (4.10.c)$$

$$[d^{+}_{j-\sigma}, H] = -(E_j + U\langle n_\sigma \rangle) d^{+}_{j-\sigma} - \Delta^{*}_{g} d_{j\sigma} - \sum_{\ell} V_{j\ell} c^{+}_{\ell-\sigma}. \qquad (4.10.d)$$

Substituting the commutation relation(4.10.a) and(4.10.b) into the Eq.(4.5) for the Green's function $G(k,k')$, we get

$$\hat{G}(k,k') = \frac{1}{2\pi}\hat{G}_o(k)\delta_{kk'} + \sum_j \hat{G}_o(k)\hat{V}(k,j)\hat{M}(j,k) \,, \qquad (4.11)$$

where the matrices $G(k,k')$, $G_0(k)$, $V(k,j)$ and $M(j,k)$ are defined as

$$\hat{G}(k,k') = \begin{pmatrix} \langle\langle c_{k\sigma}; c^{+}_{k'\sigma}\rangle\rangle & \langle\langle c_{k\sigma}; c_{-k'-\sigma}\rangle\rangle \\ \langle\langle c^{+}_{-k'-\sigma}; c^{+}_{k'\sigma}\rangle\rangle & \langle\langle c^{+}_{-k-\sigma}; c_{-k'-\sigma}\rangle\rangle \end{pmatrix}, \qquad (4.12)$$

$$\hat{G}_o(k)^{-1} = \begin{pmatrix} \omega-\epsilon_k & 0 \\ 0 & \omega+\epsilon_k \end{pmatrix}, \qquad (4.13)$$

$$\hat{V}(kj) = \begin{pmatrix} V_{jk} & 0 \\ 0 & -V^{*}_{-kj} \end{pmatrix}, \qquad (4.14)$$

and

$$\hat{M}(j,k) = \begin{pmatrix} \langle\langle d_{j\sigma}; c^{+}_{k\sigma}\rangle\rangle & \langle\langle d_{j\sigma}; c_{-k-\sigma}\rangle\rangle \\ \langle\langle d^{+}_{j-\sigma}; c^{+}_{k\sigma}\rangle\rangle & \langle\langle d^{+}_{j-\sigma}; c_{-k-\sigma}\rangle\rangle \end{pmatrix}. \qquad (4.15)$$

The matrix Green's function $\hat{M}(j,k)$ is obtained by substituting the commutation relation(4.10.c) and(4.10.d) into the equation(4.5) for $\hat{M}(j,k)$. The results of these substitutions is the new matrix equation

$$[\hat{M}_o(j)]^{-1}\hat{M}(j,k) = \sum_\ell V^{+}(j,\ell)\,\hat{G}(\ell,k) \,, \qquad (4.16)$$

where

$$\left[\hat{M}_o(j)\right]^{-1} = \begin{pmatrix} \omega - E_j - U\langle n_\sigma\rangle & \Delta_g \\ \Delta_g^* & \omega + E_j + U\langle n_\sigma\rangle \end{pmatrix}, \quad (4.17)$$

where $\overset{+}{V}(1,j)$ is the complex conjugate of the matrix(4.14). Substituting the matrix equation(4.11) into the matrix equation(4.16), we obtain

$$\left[\hat{M}_o(j)\right]^{-1}\hat{M}(j,k) = \frac{1}{2\pi}\overset{+}{V}(k,j)\hat{G}_o(k) + \sum_{j,k}|V(jk)|^2\hat{G}_o(k)M(jk). \quad (4.18)$$

To obtain the above, we have used the fact that $V(k,j)$ and $G_o(k)$ commute with each other since they are both diagonal matrices. Substituting the matrix equation(4.18) into the equation(4.11), we get

$$\hat{G}(k,k') = \frac{1}{2\pi}\hat{G}_o(k)\delta_{kk'} + \sum_j \hat{G}_o(k)\hat{V}(kj)\frac{1}{2\pi}\hat{M}'_o\,\hat{V}^+(k'j)\hat{G}_o(k')$$
$$+ \sum_j \hat{G}_o(k)\hat{V}(kj)\frac{1}{2\pi}\hat{M}'_o(j)\sum_{j'\neq j}\sum_{\ell}|V_{\ell j'}|^2\hat{G}_o(\ell)\hat{M}'_o(j')$$
$$\times \overset{+}{V}(\ell',j)\hat{G}_o(k') + \text{higher order terms}, \quad (4.19)$$

where

$$\left[\hat{M}'_o(j)\right]^{-1} = \left[\hat{M}_o(j)\right]^{-1} - \sum_{\ell}|V(\ell,j)|^2\hat{G}_o(\ell). \quad (4.20)$$

The matrix equation(4.19) can be rewritten in the form of a Dyson equation[21]

$$\left[\hat{G}(k,k')\right]^{-1} = \left[\hat{G}_o(k)\right]^{-1} - \Pi(k,k'), \quad (4.21)$$

where $\Pi(k,k')$ is the energy correction

$$\Pi(k,k') = \frac{1}{2\pi}\sum_j \hat{V}(kj)\,\hat{M}_o'(j)\,V^{+}(jk)\,. \tag{4.22}$$

Letting M_{11}, M_{12}, M_{21}, and M_{22} be the elements of $\hat{M}_o'(j)$, i.e.,

$$\hat{M}_o'(j) = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}, \tag{4.23}$$

the energy correction matrix is

$$\Pi(k,k') = \frac{1}{2\pi}\sum_j \begin{pmatrix} |V_{kj}|^2 M_{11} & -V_{kj}V^{*}_{j-k'}M_{12} \\ -V_{kj}V_{j-k}M_{21} & |V_{-kj}|^2 M_{22} \end{pmatrix}. \tag{4.24}$$

Substituting (4.24) into (4.21), we find that the inverse of the matrix Green's function $\hat{G}(k,k')$ is

$$\left[\hat{G}(k,k')\right]^{-1} = \begin{pmatrix} \omega-\epsilon_k-\frac{1}{2\pi}\sum_j|V_{kj}|^2M_{11} & \frac{1}{2\pi}\sum_j|V_{kj}|^2M_{12} \\ \frac{1}{2\pi}\sum_j|V_{kj}|^2M_{21} & \omega+\epsilon_k-\frac{1}{2\pi}\sum_j|V_{kj}|^2M_{22} \end{pmatrix}, \tag{4.25}$$

where we have assumed $\hat{V}_{kj} = \hat{V}^{*}_{-k,j}$. Inverting (4.25), we get

$$\hat{G}(k,k') = \frac{1}{\mathrm{Det}\,\hat{G}^{-1}}\begin{pmatrix} \omega+\epsilon_k-\frac{1}{2\pi}\sum_j|V_{kj}|^2M_{22} & -\frac{1}{2\pi}\sum_j|V_{kj}|^2M_{21} \\ -\frac{1}{2\pi}\sum_j|V_{kj}|^2M_{12} & \omega-\epsilon_k-\frac{1}{2\pi}\sum_j|V_{kj}|^2M_{11} \end{pmatrix}, \tag{4.26}$$

where

$$\mathrm{Det}\,G^{-1} = \Big(\omega - \epsilon_k - \frac{1}{2\pi}\sum_j |V_{kj}|^2 M_{11}\Big)\Big(\omega + \epsilon_k - \frac{1}{2\pi}\sum_j |V_{kj}|^2 M_{22}\Big)$$

$$- \frac{1}{4\pi^2}\sum_j |V_{kj}|^4 M_{21} M_{12} \;. \qquad (4.27)$$

Since

$$[M'_o(j)]^{-1} = \begin{pmatrix} \omega - E_j - U\langle n_6\rangle - \sum_\ell \frac{|V_{\ell j}|^2}{\omega - \epsilon_\ell} & \\ \Delta_g^* & \omega + E_j + U\langle n_6\rangle - \sum_\ell \frac{|V_{\ell j}|^2}{\omega + \epsilon_\ell} \end{pmatrix} \qquad (4.28)$$

we find that

$$M_{11} = \frac{\omega + E_j + U\langle n_6\rangle - \sum_\ell \frac{|V_{\ell j}|^2}{\omega + \epsilon}}{\det[\hat{M}'_o]^{-1}} , \qquad (4.29.a)$$

$$M_{12} = \frac{-\Delta_g^*}{\det[\hat{M}'_o]^{-1}} , \qquad (4.29.b)$$

$$M_{21} = \frac{-\Delta_g}{\det[\hat{M}'_o]^{-1}} , \qquad (4.29.c)$$

and

$$M_{22} = \frac{\omega - E_j - U\langle n_6\rangle - \sum_\ell \frac{|V_{\ell j}|^2}{\omega - \epsilon}}{\det[\hat{M}'_o]^{-1}} , \qquad (4.29.d)$$

where

$$\det[\hat{M}_0']^{-1} = (\omega + E_j + U\langle n_\sigma\rangle + \sum_{\ell} \frac{|V_{\ell j}|^2}{\omega+\epsilon})(\omega - E_j - U\langle n_\sigma\rangle - \sum_{\ell} \frac{|V_{\ell j}|^2}{\omega-\epsilon})$$

$$-|\Delta_g|^2 . \qquad (4.30)$$

By assuming that V_{jl} is a constant and by replacing the summation over l by an integration over d^3l, the above equations (4.29.a) to (4.29.d) become

$$M_{11} = \frac{\omega + B}{\omega^2 - B^2 - \Delta_g^2}, \qquad (4.31.a)$$

$$M_{12} = \frac{-\Delta_g^*}{\omega^2 - B^2 - \Delta_g^2}, \qquad (4.31.b)$$

$$M_{21} = \frac{-\Delta_g}{\omega^2 - B^2 - \Delta_g^2}, \qquad (4.31.c)$$

$$M_{22} = \frac{\omega - B}{\omega^2 - B^2 - \Delta_g^2}, \qquad (4.31.d)$$

where

$$B = E_j + U\langle n_\sigma\rangle + \frac{2m P_F V^2}{(2\pi)^3} \ln \frac{\omega - \omega_D}{\omega + \omega_D} . \qquad (4.32)$$

Because the integral diverges, a cut-off at the Debye frequency has been introduced.