6 Methods of Green's Functions

Let us work in the unit in which Plank's constant is measured to be one, $\hbar = 1$.

6.1 Pictures of quantum dynamics

6.1.1 Schrodinger picture

Let $|\psi(t)\rangle$ be a time dependent state vector of quantum system, satisfy Schrodinger's equation

$$i\partial_t|\psi(t)\rangle = H|\psi(t)\rangle \tag{6.1}$$

where $H \neq H(t)$ is the system Hamiltonian, normally time independent for stationary system. Let $O = O(, x, p)$ be an operator of any physics property of the system, its quantum expectation value is

$$\langle O\rangle(t) = \langle\psi(t)|O|\psi(t)\rangle \tag{6.2}$$

It is normally time dependent according to the state vector. This is or familiar form of quantum calculation, it is called *Schrodinger picture*, characterize by time dependent state vector $|\psi(t)\rangle_S$ and time-independent physical operator O_S, where the subscribe S is added for clarity.

6.1.2 Heisenberg picture

Let us define time-evolution operator $U(t, 0)$, applied on the Schrodinger state vector as

$$|\psi(t)\rangle_S = U(t, 0)|\psi(0)\rangle_S \tag{6.3}$$

Apply to (6.1), we get

$$i\partial_r U(t, 0) = HU(t, 0) \to U(t, 0) = e^{-iHt}, \text{ with } U(0, 0) = 1 \tag{6.4}$$

This show that $U(t, 0)$ is unitary operator. Apply to (6.2), we have

$$\langle O\rangle(t) = {}_S\langle\psi(0)|U^\dagger(t, 0)O_S U(t, 0)|\psi(0)\rangle_S = {}_H\langle\psi|O_H(t)|\psi\rangle_H \tag{6.5}$$

where we have define Heisenberg picture of state vector and operator as

$$|\psi\rangle_H = |\psi(0)\rangle_S, \quad O_H(t) = U^\dagger(t, 0)O_S U(t, 0) \tag{6.6}$$

From this assignment we observe that

$$i\partial_t O_H(t) = -HO_H(t) + O_H(t)H = [O_H(t), H] \tag{6.7}$$

This is called *Heisenberg's equation.* So that in Heisenberg picture, dynamics of quantum system appear in an operator, with static state vector.

6.1.3 Interaction picture

In case of the interacting system where the separation of the system Hamiltonian can be done as

$$H(t) = H_0 + V \tag{6.8}$$

Let us define the time evolution operator $U_0(t, 0)$ and define the interacting state vector as

$$U_0(t,0) = e^{-iH_0 t} \to |\psi(t)\rangle_S = U_0(t,0)|\psi(t)\rangle_I \tag{6.9}$$

$$(6.1) \to i\partial_t|\psi(t)\rangle_t = V_I(t)|\psi(t)\rangle_I \tag{6.10}$$

where the interacting picture of quantum operator is defined from the Schrodinger operator as

$$O_I(t) = U_0^\dagger(t,0)O_S U_0(t,0) = U_0^\dagger(t,0)U(t,0)O_H(t)U^\dagger(t,0)U_0(t,0) \tag{6.11}$$

$$= U_I(t,0)O_H(t)U_I^\dagger(t,0), \text{ where } U_I(t,0) = U_0^\dagger(t,0)U(t,0) \tag{6.12}$$

From (6.11), we have

$$i\partial_t O_I(t) = -H_0 O_I(t) + O_I(t)H_0 = [O_I(t), H_0] \tag{6.13}$$

From (6.12), we will have

$$\begin{aligned} i\partial_t U_I(t,0) &= -H_0 U_0^\dagger(t,0)U(t,0) + U_0^\dagger(t,0)HU(t,0) \\ &= V_I(t)U_I(t,0) \end{aligned} \tag{6.14}$$

By direct integration, with some iterations, we get

$$U_I(t,0) = 1 - i\int^t dt' V_I(t')U_I(t',0) \tag{6.15}$$

$$= 1 - i\int^t dt' V_I(t') + (-i)^2 \int^t dt' \int^{t'} dt'' V_I(t')V_I(t'') + ... \tag{6.16}$$

Using identity

$$\int^t dt' \int^{t'} dt'' V_I(t')V_I(t'') = \frac{1}{2}\int^t dt' \int^t dt'' T[V_I(t')V_I(t'')] \tag{6.17}$$

and generalize to

$$\begin{aligned} &\int^t dt_1 \int^{t_1} dt_2 ... \int^{t_{n-1}} dt_n V_I(t_1)...V_I(t_n) \\ &= \frac{1}{n!}\int^t dt_1 \int^t dt_2 ... \int^t dt_n T[V_I(t_1)...V_I(t_n)] \end{aligned} \tag{6.18}$$

where T is *time-ordering operator*. From (6.16), we will have

$$\begin{aligned} U_I(t,0) &= 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int^t dt_1 ... \int^t dt_n T[V_I(t_1)...V_I(t_n)] \\ &= T\exp\left\{-i\int^t dt' V_I(t')\right\} \end{aligned} \tag{6.19}$$

6.2 Many-body Green's functions

Let $\psi(x,t)$ be second quantized state function operator, it is born to be Heisenberg operator, and derived from Schrodinger equation in the first quantization. The casual Green function is defined in term of the time-ordered product of state function operator as

$$iG(x,t;x',t') = \frac{\langle\Omega|T[\psi(x,t)\psi^\dagger(x',t')]|\Omega\rangle}{\langle\Omega|\Omega\rangle} \tag{6.20}$$

where $|\Omega\rangle$ is the ground state (numbering) of the system. For non-interacting system we have $\langle\Omega_0|\Omega_0\rangle = 1$, and

$$\begin{aligned} iG_0(x,t;x',t') &= \langle\Omega_0|T[\psi(x,t)\psi^\dagger(x',t']|\Omega_0\rangle & (6.21) \\ &= \theta(t-t')\langle\Omega_0|\psi(x,t)\psi^\dagger(x',t')|\Omega_0\rangle \\ &\quad \pm\theta(t'-t)\langle\Omega_0|\psi^\dagger(x',t')\psi(x,t)|\Omega_0\rangle & (6.22) \\ &= G^>(x,t;x',t') \pm G^<(x,t;x',t') & (6.23) \end{aligned}$$

where the $(+)$ signe is for bosonic operators, while the $(-)$ sign is for fermionic operators. They are called greater and lesser Green's function, respectively. We also have retarded and advanced Green's functions, which are defined as

$$G^R(x,t;x',t') = \theta(t-t')\langle\Omega_0|[\psi(x,t),\psi^\dagger(x',t')]_\mp|\Omega_0\rangle \tag{6.24}$$

$$G^A(x,t;x',t') = -\theta(t'-t)\langle\Omega_0|[\psi(x,t),\psi^\dagger(x',t')]_\mp|\Omega_0\rangle \tag{6.25}$$

They are related to the greater and lesser Green's functions as

$$G^R(x,t;x',t') = \theta(t-t')\left(G^>(x,t;x',t') - G^<(x,t;x',t')\right) \tag{6.26}$$
$$G^A(x,t;x',t') = -\theta(t'-t)\left(G^<(x,t;x',t') - G^>(x,t;x',t')\right) \tag{6.27}$$

For more convenient let us assign $t = t$, $t' = 0$, and we also denote $\psi(x,0) = \psi(x)$. Applying the expansion

$$\psi(x,t) = \frac{1}{\sqrt{V}}\sum_k a_k(t)e^{ik\cdot x} \tag{6.28}$$

From above we will have

$$\begin{aligned} iG_0(x,x';t) = \frac{1}{V}\sum_k e^{ik\cdot(x-x')}\Big(&\theta(t)\langle\Omega_0|a_k(t)a_{k'}^\dagger(0)|\Omega_0\rangle \\ &\pm\theta(-t)\langle\Omega_0|a_{k'}^\dagger(0)a_k(t)|\Omega_0\rangle\Big) \qquad (6.29)\\ &\equiv i\int\frac{d^3k}{(2\pi)^3}e^{ik\cdot(x-x')}G_0(k,t) \qquad (6.30)\end{aligned}$$

Then we have

$$iG_0(k,t) = \theta(t)\langle\Omega_0|a_k(t)a_{k'}^\dagger(0)|\Omega_0\rangle \pm \theta(-t)\langle\Omega_0|a_{k'}^\dagger(0)a_k(t)|\Omega_0\rangle \tag{6.31}$$

Let us apply to simple systems.

6.2.1 Free fermions

We have

$$H = \sum_k \xi_k c_k^\dagger c_k,\ \{c_k, c_{k'}^\dagger\} = \delta_{kk'} \tag{6.32}$$
$$i\partial_t c_k(t) = [c_k(t), H] = \xi_k c_k(t) \to c_k(t) = e^{-i\xi_k t}c_k \tag{6.33}$$
$$\begin{aligned}(6.31) \to iG(k,t) &= \theta(t)e^{-i\xi_k t}\langle\Omega_0|c_k c_k^\dagger|\Omega_0\rangle - \theta(-t)e^{-i\xi_k t}\langle\Omega_0|c_k^\dagger c_k|\Omega_0\rangle \\ &= \theta(t)e^{-i\xi_k t}(1-n_k) - \theta(-t)e^{-i\xi_k t}n_k \qquad (6.34)\end{aligned}$$

with

$$n_k = \langle\Omega_0|c_k^\dagger c_k|\Omega_0\rangle = \begin{cases} 1, & k \le k_F \\ 0, & k > k_F \end{cases} \tag{6.35}$$

Using identity

$$\theta(\pm t) = \lim_{\eta\to 0}\frac{\pm i}{2\pi}\int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega \mp i\eta}$$

And apply the Fourier transformation of the Green's function

$$G(k,t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} G(k,\omega) \tag{6.36}$$

$$G(k,\omega) = \frac{1-n_k}{\omega - \xi_k + i\eta} - \frac{n_k}{\omega - \xi_k - i\eta} \tag{6.37}$$

From above we have

$$G^{>}(k,\omega) = \frac{1-n_k}{\omega - \xi_k + i\eta},\ G^{<}(k,\omega) = -\frac{n_k}{\omega - \xi_k - i\eta} \tag{6.38}$$

$$G^{R}(k,\omega) = \frac{1}{\omega - \xi_k + i\eta},\ G^{A}(k,\omega) = \frac{1}{\omega - \xi_k - i\eta} \tag{6.39}$$

6.2.2 Free bosons

We have

$$H = \sum_q \omega_q b_q^\dagger b_q,\ [b_q, b_{q'}^\dagger] = \delta_{qq'} \tag{6.40}$$

$$i\partial_t b_q(t) = [b_q(t), H] = \omega b_q(t) \to b_q(t) = e^{-i\omega_q t},\ b_q^\dagger(t) = e^{i\omega_q t} b_q^\dagger \tag{6.41}$$

$$\begin{aligned} \phi_q = b_q + b_{-q}^\dagger \to \phi_q \phi_q^\dagger &= (b_q + b_{-q}^\dagger)(b_q^\dagger + b_{-q}) \\ &= b_q b_q^\dagger + b_{-q}^\dagger b_{-q} + b_{-q}^\dagger b_q^\dagger + b_q b_{-q} \end{aligned} \tag{6.42}$$

From (6.31), we have

$$\begin{aligned} D^{>}(q,t) &= \theta(t)\langle\Omega_0|\phi_q(t)\phi_q^\dagger(0)|\Omega\rangle \\ &= \theta(t)\left(\langle\Omega_0|b_q(t)b_q^\dagger(0)|\Omega_0\rangle + \langle\Omega_0|b_{-q}^\dagger(t)b_{-q}(0)|\Omega_0\rangle\right) \\ &= \theta(t)\left(e^{-i\omega_q t}(1+n_q) + e^{i\omega_q t} n_q\right) \end{aligned} \tag{6.43}$$

After we have used the fact that $\omega_{-q} = \omega_q$ and $n_{-q} = n_q$. Apply its Fourier transformation, we have

$$D^{>}(q,\omega) = \frac{1+n_q}{\omega - \omega_q + i\eta} + \frac{n_q}{\omega + \omega_q + i\eta} \tag{6.44}$$

Similar analysis we can have

$$D^{<}(q,\omega) = \frac{n_q}{\omega - \omega_q - i\eta} + \frac{1+n_q}{\omega + \omega_q - i\eta} \tag{6.45}$$

And we will have

$$D^{R}(q,\omega) = \frac{1}{\omega - \omega_q + i\eta} - \frac{1}{\omega + \omega_q + i\eta} = \frac{2\omega_q}{\omega^2 - \omega_q^2} \tag{6.46}$$

$$D^{A}(q,\omega) = \frac{1}{\omega - \omega_q - i\eta} - \frac{1}{\omega + \omega_q - i\eta} = \frac{2\omega_q}{\omega^2 - \omega_q^2} \tag{6.47}$$

6.3 Spectral representation

For a system of N-fermions, we will have $|\Omega_0^N\rangle$ as its ground state with energy E_0^N. The fermionic Green's function is then read

$$\begin{aligned}
iG_0(k,t) &= \theta(t)\langle\Omega_0^N|a_k(t)a_k^\dagger(0)|\Omega_0^N\rangle \\
&\quad -\theta(-t)\langle\Omega_0^N|a_k^\dagger(0)a_k(t)|\Omega_0^N\rangle && (6.48)\\
&= \theta(t)\sum_n\langle\Omega_0^N|a_k(t)|\Omega_n^{N+1}\rangle\langle\Omega_n^{N+1}|a_k^\dagger(0)|\Omega_0^N\rangle \\
&\quad -\theta(-t)\sum_n\langle\Omega_0^N|a_k^\dagger(0)|\Omega_n^{N-1}\rangle\langle\Omega_n^{N-1}|a_k(t)|\Omega_0^N\rangle && (6.49)\\
&= \theta(t)\sum_n\langle\Omega_0^N|e^{iHt}a_k(0)e^{-iHt}|\Omega_n^{N+1}\rangle\langle\Omega_n^{N+1}|a_k^\dagger(0)|\Omega_0^N\rangle \\
&\quad -\theta(-t)\sum_n\langle\Omega_0^N|a_k^\dagger(0)|\Omega_n^{N-1}\rangle\langle\Omega_n^{N-1}|e^{iHt}a_k(0)e^{-iHt}|\Omega_0^N\rangle && (6.50)\\
&= \theta(t)\sum_n e^{-i(E_n^{N+1}-E_0^N)t}\langle\Omega_0^N|a_k(0)|\Omega_n^{N+1}\rangle\langle\Omega_n^{N+1}|a_k^\dagger(0)|\Omega_0^N\rangle \\
&\quad -\theta(-t)\sum_n e^{i(E_n^{N-1}-E_0^N)t}\langle\Omega_0^N|a_k^\dagger(0)|\Omega_n^{N-1}\rangle\langle\Omega_n^{N-1}|a_k(0)|\Omega_0^N\rangle && (6.51)\\
&= \theta(t)\sum_n e^{-i(E_n^{N+1}-E_0^N)t}|\langle\Omega_n^{N+1}|a_k^\dagger|\Omega_0^N\rangle|^2 \\
&\quad -\theta(-t)\sum_n e^{i(E_n^{N-1}-E_0^N)t}|\langle\omega_0^N|a_k^\dagger|\Omega_n^{N-1}\rangle|^2 && (6.52)
\end{aligned}$$

Apply Fourier transformation, we have

$$G(k,\omega)=\sum_n\left(\frac{|\langle\Omega_n^{N+1}|a_k^\dagger|\Omega_0^N\rangle|^2}{\Omega-(E_n^{N+1}-E_0^N)+i\eta}+\frac{|\langle\Omega_0^N|a_k^\dagger|\Omega_n^{N-1}\rangle|^2}{\omega+(E_n^{N-1}-E_0^N)-i\eta}\right) \tag{6.53}$$

Now let us define

$$E_n^{N+1}-E_0^N=(E_n^{N+1}-E_0^{N+1})+(E_0^{N+1}-E_0^N)=\epsilon_k+\mu,\ \ k>k_F \tag{6.54}$$
$$E_n^{N_1}-E_0^N=(E_n^{N_1}-E_0^{N-1})-(E_0^N-E_0^{N-1})=\epsilon_k-\mu,\ \ k\le k_F \tag{6.55}$$

Then define spectral functions

$$A(k,\omega)=\sum_n|\langle\Omega_n^{N+1}|a_k^\dagger|\Omega_0^N\rangle|^2\delta(\omega-\epsilon_k-\mu)=\delta(\omega-\epsilon_k-\mu) \tag{6.56}$$
$$B(k,\omega)=\sum_n|\langle\Omega_0^N|a_k^\dagger|\Omega_n^{N-1}\rangle|^2\delta(\omega-\epsilon_k+\mu)=\delta(\omega-\epsilon_k+\mu) \tag{6.57}$$

for non-interacting fermions. One can write the fermionic Green's function in its spectral representation as

$$G(k,\omega) = \int d\omega' \left(\frac{A(k,\omega')}{\omega - \omega' + i\eta} - \frac{B(k,\omega')}{\omega - \omega' - i\eta} \right) \tag{6.58}$$

From the identity

$$\frac{1}{x \pm i\eta} = P\left(\frac{1}{x}\right) \pm i\pi\delta(x)$$

We observe that

$$A(k,\omega) = \frac{1}{\pi} ImG^{>}(k,\omega) \tag{6.59}$$

$$B(k,\omega) = \frac{1}{\pi} ImG^{<}(k,\omega) \tag{6.60}$$

These are generic form of contribution of spectral function in the Green's function. From Kramer-Kronig relation we will have

$$\mathrm{Re}G(k,\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} d\omega' \frac{\mathrm{Im}G(k,\omega')}{\omega - \omega'} \tag{6.61}$$

$$\mathrm{Im}G(k,\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} d\omega' \frac{\mathrm{Re}G(k,\omega')}{\omega - \omega'} \tag{6.62}$$

6.4 Thermal Green's function

Let there be thermal operator

$$\rho = e^{-\beta H}, \ \beta = \frac{1}{k_B T}, \ \to Z = Tre^{-\beta H} \tag{6.63}$$

$$\langle\langle O \rangle\rangle = \frac{1}{Z} Tr[\rho O] \tag{6.64}$$

Thermal Green's function is defined by first applying *Wick's rotation* of the real to imaginary time $t \to -i\tau$, so that the quantum Heisenberg operator will changed to be

$$a_k(t) = e^{iHt} a_k e^{-iHt} \to a_k(\tau) = e^{\tau H} a_k e^{-\tau H} \tag{6.65}$$

And thermal Green's function is defined in the form

$$\mathcal{G}(k;\tau,\tau') = -\langle\langle T_\tau [a_k(\tau) a_k^\dagger(\tau')] \rangle\rangle \tag{6.66}$$

In general, $\mathcal{G}(k;\tau,\tau') = \mathcal{G}(k;\tau - \tau')$, since

$$\tau, \tau' \in [0,\beta] \to \tau - \tau' \in [-\beta, \beta]$$

And there will be (periodicity/anti-periodicity) of (bosonic/fermionic) thermal Green's function. Let us determine, for $\tau - \beta > 0$,

$$\mathcal{G}(k; \tau - \beta) = -\frac{1}{Z} Tr \left[a_k(\tau - \beta) a_k^\dagger(0) \right] \tag{6.67}$$

6.5 Matsubara frequencies