1 Green's Functions

Let $\varphi(x,t)$ be second quantized state function operator, staisfy Heisenberg equation

$$i\partial_t\varphi(x,t) = [\varphi(x,t), H]$$

where H is system Hamiltonian, normally in second quantized form. The many-body Green's function will be constructed from $\varphi(x,t)$, and perturbation theory will be developed for the interaction, with diagrammatic approach.

1.1 Definition

The *causal Green's function* is define as

$$iG(x,t;x',t') = \langle T[\varphi(x,t)\varphi^\dagger(x',t')]\rangle \tag{1}$$

$$= \theta(t-t')\langle\varphi(x,t)\varphi^\dagger(x',t')\rangle \pm \theta(t'-t)\langle\varphi^\dagger(x',t')\varphi(x,t)\rangle \tag{2}$$

$$= iG^>(x,t;x',t') \pm iG^<(x,t;x',t') \tag{3}$$

where $\langle ...\rangle$ is quantum expectation with respect to system ground state, T is time ordering operator, and $\pm$ signs result from bosonic/fermionic operators, respectively.

The *retarded* and *advanced Green's functions* are defined as

$$iG^R(x,t;x',t') = \theta(t-t')\langle[\varphi(x,t),\varphi^\dagger(x',t')]_\mp\rangle \tag{4}$$

$$iG^A(x,t;x',t') = \theta(t'-t)\langle[\varphi(x,t),\varphi^\dagger(x',t')]_\mp\rangle \tag{5}$$

where $[...]_\mp$ means commutator/anti-commutator for bosonic/fermionic operators, respectively.

The causal Green's function is suitable for doing formulation, especially of perturbation theory, while the retarded Green's function has many applications in condensed matter theories. They are related as

$$G^R(x,t;x',t') = \theta(t-t')\left(G^>(x,t;x',t') - G^<(x,t;x',t')\right) \tag{6}$$

1.2 Non-interacting Green's function

Let us determine the retarded Green's function from (4), and apply with the expansion

$$\varphi(x,t) = \sum_k a_k(t)\phi_k(x),\ \phi_k(x) = \frac{1}{\sqrt{V}}e^{ik\cdot x} \tag{7}$$

$$\to iG^R(x,t;x',t') = \theta(t-t')\frac{1}{V}\sum_{k,k'} e^{ik\cdot x - ik'\cdot x'}\langle[a_k(t), a^\dagger_{k'}(t')]_\mp\rangle \tag{8}$$

Let us define

$$iG^R(x,t;x',t') = \frac{1}{V}\sum_{k,k'} e^{ik\cdot x - ik'\cdot x'} iG^R_{kk'}(t-t') \tag{9}$$

$$\rightarrow iG^R_{kk'}(t-t') = \theta(t-t')\langle[a_k(t), a^\dagger_{k'}(t')]_\mp\rangle \tag{10}$$

1.2.1 Free fermions

Here we have

$$H = \sum_k \xi_k c^\dagger_k c_k,\ \xi_k = \epsilon_k - \mu,\ \{c_k, c^\dagger_{k'}\} = \delta_{kk'} \tag{11}$$

$$c_k(T) = e^{iHt}c_k e^{-iHt} \rightarrow i\partial_t c_k(t) = [c_k(t), H] = \xi_k c_k(t) \tag{12}$$

$$\rightarrow c_k(t) = e^{-i\xi_k t}c_k,\ c^\dagger_k(t) = e^{i\xi_k t}c^\dagger_k \tag{13}$$

From (10) we have

$$\begin{aligned} iG^R_{kk,}(t-t') &= \theta(t-t')e^{-i\xi_k t + ixi_{k'}t'}\langle\{c_k, c^\dagger_{k'}\}\rangle \\ &= \theta(t-t')e^{-i\xi_k(t-t')}\delta_{kk'} = iG^R(k, t-t')\delta_{kk'} \end{aligned} \tag{14}$$

Using identity

$$\theta(t-t') = \frac{i}{2\pi}\int d\omega \frac{e^{-i\omega(t-t')}}{\omega + i\eta},\ \eta \rightarrow 0^+$$

and apply the Fourier transformation

$$iG^R(k, t-t') = \frac{i}{2\pi}\int d\omega e^{-i\omega(t-t')}G^R(k,\omega) \tag{15}$$

$$\rightarrow G^R(k,\omega) = \frac{1}{\omega - \xi_k + i\eta} \tag{16}$$

1.2.2 Free bosons

Here we have

$$H = \sum_q \omega_q b^\dagger_q b_q,\ [b_q, b^\dagger_{q'}] = \delta_{qq'} \tag{17}$$

$$b_q(t) = e^{iHt}b_q e^{-iHt} \rightarrow i\partial_t b_q(t) = [b_q(t), H] = \omega_q b_q(t) \tag{18}$$

$$\rightarrow b_q(t) = e^{-i\omega_q t}b_q,\ b^\dagger_q(t) = e^{i\omega_q t}b^\dagger_q \tag{19}$$

$$a_q = b_q + b^\dagger_{-q}, a^\dagger_q = b^\dagger_q + b_{-q} \rightarrow [a_q, a^\dagger_{q'}] = [b_q, b^\dagger_{q'}] + [b^\dagger_{-q}, b_{-q'}] \tag{20}$$

From (10), with a bit change of notation, we have

$$\begin{aligned} iD^R_{qq'}(t-t') &= \theta(t-t')\left(e^{-i\omega_q t+i\omega_{q'}t'}\langle[b_q,b^\dagger_{q'}]\rangle + e^{i\omega_q t-i\omega_{q'}t'}\langle[b^\dagger_{-q},b_{-q'}]\rangle\right) \\ &= \theta(t-t')\left(e^{-i\omega_q(t-t')} - e^{i\omega_q(t-t')}\right)\delta_{qq'} = iD^R(k,t-t')\delta_{qq'} \quad (21) \end{aligned}$$

Apply the Fourier transformation, and using identity of the step function, we have

$$iD^R(q,t-t') = \frac{i}{2\pi}\int d\omega e^{-i\omega(t-t')}D^R(q,\omega) \quad (22)$$

$$D^R(q,\omega) = \frac{1}{\omega-\omega_q+i\eta} - \frac{1}{\omega+\omega_q+i\eta} = \frac{2\omega_q}{\omega^2-\omega_q^2} \quad (23)$$

1.3 Spectral functions

Let us define $|\psi_0^N\rangle$ be a ground state of N-fermions system, from (10), we can have

$$\begin{aligned} iG^R(k,t-t') &= \theta(t-t')\langle\psi_0^N|\{c_k(t),c_k^\dagger(t')\}|\psi_0^N\rangle \\ &= \theta(t-t')\left(\langle\psi_0^N|c_k(t)c_k^\dagger(t')|\psi_0^N\rangle + \langle\psi_0^N|c_k^\dagger(t')c_k(t)|\psi_0^N\rangle\right) \\ &= \theta(t-t')\sum_n\Big(\langle\psi_0^N c_k(t)|\psi_n^{N+1}\rangle\langle\psi_n^{N+1}|c_k^\dagger(t')|\psi_0^N\rangle \\ &\qquad + \langle\psi_0^N|c_k^\dagger(t')|\psi_n^{N-1}\rangle\langle\psi_n^{N-1}|c_k(t)|\psi_0^N\rangle\Big) \\ &= \theta(t-t')\sum_n\Big(e^{-i(E_n^{N+1}-E_0^N)(t-t')}|\langle\psi_n^{N+1}|c_k^\dagger|psi_0^N\rangle|^2 \\ &\qquad + e^{-i(E_n^{N-1}-E_0^N)(t'-t)}|\langle\psi_0^N|c_k^\dagger|\psi_n^{N-1}\rangle|^2\Big) \quad (24) \end{aligned}$$

Apply with Fourier transformation, we have

$$G^R(k,\omega) = \sum_n\left(\frac{|\langle\psi_n^{N+1}|c_k^\dagger|\psi_0^N\rangle|^2}{\omega-(E_n^{N-1}-E_0^N)+i\eta} + \frac{|\langle\psi_0^N|c_k^\dagger|\psi_n^{N-1}\rangle|^2}{\omega+(E_n^{N-1}-E_0^N)+i\eta}\right) \quad (25)$$

Note that

$$E_n^{N+1}-E_0^N = (E_n^{N+1}-E_0^{N+1}) + (E_0^{N+1}-E_0^N) = \epsilon_k+\mu \quad (26)$$

$$E_n^{N-1}-E_0^N = (E_n^{N-1}-E_0^{N-1}) - (E_n^N-E_0^{N-1}) = \epsilon_k-\mu \quad (27)$$

Let us define *spectral function*

$$\rho(k,\omega) = \sum_n |\psi_n^{N+1}|c_k^\dagger|\psi_0^N\rangle|^2\delta(\omega - \epsilon_k - \mu) + \sum_n |\langle\psi_0^N|c_k^\dagger|\psi_n^{N-1}\rangle|^2\delta(\omega - \epsilon + \mu) \tag{28}$$

Then we have from (25)

$$G^R(k,\omega) = \int d\omega' \frac{\rho(k,\omega')}{\omega - \omega' + i\eta} \tag{29}$$

For free fermions we have $\rho(k, \omega = \delta(\omega - \xi_k)$. From identity

$$\frac{1}{x + i\eta} = P\left(\frac{1}{x}\right) - i\pi\delta(x) \to \rho(k,\omega) = -\frac{1}{\pi} Im G^R(k,\omega) \tag{30}$$

1.4 Thermal averaged Green's function

Let there be statistical operator

$$\rho = e^{-\beta K},\ \beta = \frac{1}{k_B T},\ K = H - \mu N \tag{31}$$

$$\to Z = Tr[\rho] = \sum_{N,n} \langle\psi_n^N|e^{-\beta K}|\psi_n^N\rangle = \sum_{N,n} e^{-\beta(E_n^N - \mu N)} \tag{32}$$

$$\langle\langle O\rangle\rangle = \frac{1}{Z} Tr\left[\rho O\right] \equiv \frac{1}{Z}\sum_{N,n}\langle\psi_n^N|e^{-\beta K} O|\psi_n^N\rangle \tag{33}$$

Thermal averaged Green's function is defined as

$$\tilde{G}(k;t,t') = \langle\langle G(k;t,t')\rangle\rangle = -i\frac{1}{Z} Tr\left[e^{-\beta K} T[a_k(t)a_k^\dagger(t')]_\mp\right] \tag{34}$$

Apply Wick's rotation $t \to \tau = it$, so that

$$a_k(t) = e^{iKt} a_k e^{-iKt} \to a_k(\tau) = e^{K\tau} a_k e^{-K\tau}, a_k^\dagger(\tau) = e^{K\tau} a_k^\dagger e^{-K\tau} \tag{35}$$

From (34), we have

$$\tilde{G}(k;t,t') \to \mathcal{G}(k;\tau,\tau') = -\frac{1}{Z} Tr\left[e^{-\beta K}\mathcal{T}[a_k(\tau)a_k^\dagger(\tau')]\right] = -\frac{1}{Z} Tr\left[e^{-\beta K}\mathcal{T}[e^{K\tau} a_k e^{-K(\tau-\tau')} a_k^\dagger e^{-K\tau'}]\right] = -\frac{1}{Z} Tr\left[e^{-\beta K}\mathcal{T}[e^{K(\tau-\tau')} a_k e^{-K(\tau-\tau')} a_k^\dagger]\right] \equiv \mathcal{G}(k, \tau - \tau') \tag{36}$$

Now let $\tau' = 0, \tau \in [-\beta, \beta]$., from (36) we have

$$\begin{aligned}\mathcal{G}(k,\tau) &= -\frac{1}{Z}Tr\left[e^{-\beta K}\mathcal{T}[a_k(\tau)a_k^\dagger(0)]\right] \\ &= -\frac{1}{Z}Tr\left[e^{K(\tau-\beta)}a_k e^{-K\tau}a_k^\dagger\right],\ \tau > 0\end{aligned} \tag{37}$$

Note that

$$\begin{aligned}\mathcal{G}(k,\tau+\beta) = -\frac{1}{Z}Tr\left[e^{K\tau}a_k e^{-K(\tau+\beta)}a_k^\dagger\right],\ \tau > 0 \\ = -\frac{1}{Z}Tr\left[e^{-K\beta}a_k^\dagger\left(e^{K\tau}a_k e^{-K\tau}\right)\right] \\ = \pm\left(-Tr\left[e^{-\beta K}a_k(\tau)a_k^\dagger(0)\right]\right) = \pm\mathcal{G}(k,\tau)\end{aligned} \tag{38}$$

A similar result can be obtained for $\tau < 0$. We observe periodicity $\pm$ of bosnonic/fermionic thermal averaged Green's function.

Since $\tau \in [-\beta, \beta]$, we apply Fourier transformation of $\mathcal{G}(k,\tau)$ in the form

$$\mathcal{G}(k,\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{+\infty} e^{-i\nu_n\tau}\mathcal{G}(k,i\nu_n) \tag{39}$$

$$\mathcal{G}(k,i\nu_n) = \int_0^\beta d\tau e^{i\nu_n\tau}\mathcal{G}(k,\tau) \tag{40}$$

where ν_n is known as *Matsubara frequency*, is defined to capture periodicity of the thermal averaged Green's function, as

$$\nu_n\beta = \begin{cases} 2n\pi, & bosons \\ (2n+1)\pi, & fermions \end{cases} \tag{41}$$

In case of free fermions, we do have

$$H = \sum_k \xi_k c_k^\dagger c_k,\ \xi_k = \epsilon_k - \mu \tag{42}$$

$$\mathcal{G}^R(k,\tau) = -\theta(\tau)\langle\langle\{c_k(\tau), c_k^\dagger(0)\}\rangle\rangle = -\theta(\tau)e^{-\xi_k\tau} \tag{43}$$

$$\begin{aligned}\mathcal{G}(k,i\nu_n) = \int_0^\beta d\tau e^{i\nu_n\tau}\mathcal{G}(k,\tau) = -\int_0^\beta d\tau e^{i\nu_n\tau - \xi_k\tau} \\ = \frac{1}{i\nu_n - \xi_k}\end{aligned} \tag{44}$$

We observe the real to imaginary frequency, under thermal averaging, of the Green's function as

$$\omega + i\eta \to i\nu_n$$

Therefore, the thermal averaged free bosonic Green's function will appear in the form

$$\mathcal{D}(q, i\nu_n) = \frac{2\omega_q}{(i\nu_n)^2 - \omega_q^2} \tag{45}$$

1.5 Interacting system

System Hamiltonian is

$$H = H_0 + V \tag{46}$$

Define unitary operator

$$U(t) = e^{-iHt},\ U_0(t) = e^{-iH_0 t} \tag{47}$$

$$\rightarrow a_H(t) = U^{-1}(t)a(0)U(t), \tag{48}$$

$$\begin{aligned} a_I(t) = U_0^{-1}(t)a(0)U_0(t) &= U_0^{-1}(t)U(t)a_H(t)U^{-1}(t)U_0(t) \\ &= U_I(t)a_H(t)U_I^{-1}(t) \end{aligned} \tag{49}$$

$$\begin{aligned} U_I(t) = U_0^{-1}(t)U(t) = e^{iH_0 t}e^{-iHt} \rightarrow i\partial_t U_I(t) &= e^{iH_0 t}(-H_0 + H)e^{-iHt} \\ &= V_I(t)U_I(t) \end{aligned} \tag{50}$$

$$\rightarrow U_i(t) = U_I(0) + (-i)\int_0^t dt' V_I(t')U_I(t') \tag{51}$$

Solution is derived by infinite iterations. Using identity

$$\begin{aligned} &\int_0^t dt_1 \int_0^{t_1} dt_2 ... \int_0^{t_{n-1}} dt_n V_I(t_1)...V_I(t_n) \\ &= \frac{1}{n!}\int_0^t ... \int_0^t dt_1...dt_n T[V_I(t_1)...V_I(t_n)] \end{aligned} \tag{52}$$

From (51) we have

$$U_I(t) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_0^t dt_1 ... \int_0^t dt_n T[V_I(t_1)...V_I(t_n)] \tag{53}$$

$$= T\exp\left\{-i\int_0^t dt' V_I(t')\right\} \tag{54}$$

From definition of imaginary time Green's function

$$\begin{aligned} \mathcal{G}(k,\tau) = -\frac{Tr\left[\mathcal{T}[e^{-\beta K}a_k(\tau)a_k^\dagger(0)]\right]}{Tr\left[e^{-\beta K}\right]} &= -\frac{Tr\left[\mathcal{T}[e^{-\beta K}e^{K\tau}a_{Ik}(\tau)e^{-K\tau}a_{Ik}^\dagger(0)]\right]}{Tr\left[e^{-\beta K}\right]} \\ &= -\frac{Tr\left[\mathcal{T}[U_I(\beta,0)a_{I,k}(\tau)a_{I,k}^\dagger(0)]\right]}{Tr\left[U_I(\beta,0)\right]} \end{aligned} \tag{55}$$

Now let us determine

$$Tr\left[U_I(\beta,0)\right] = Tr\left[\mathcal{T}\exp\left\{-i\int_0^\beta d\tau V_I(\tau)\right\}\right] = 1+\sum_{n=1}^{\infty} D_n$$

$$D_n = \frac{(-i)^n}{n!}\int_0^\beta d\tau_1 ... \int_0^\beta d\tau_n Tr\left[\mathcal{T}[V_I(\tau_1)...V_I(\tau_n)]\right] \tag{56}$$

$$Tr\left[U_I(\beta,0)a_{I,k}(\tau)a^\dagger_{I,k}(0)\right] = Tr\left[\mathcal{T}\left(a_{I,k}(\tau)a^\dagger_{I.k}(0)\exp\left\{-i\int_0^\beta d\tau' V_I(\tau')\right\}\right)\right]$$

$$= C_0(\tau,0)+\sum_{n=1}^{\infty} C_n \tag{57}$$

$$C_0(\tau,0) = Tr\left[a_{I,k}(\tau)a^\dagger_{I,k}(0)\right] \tag{58}$$

$$C_n = \frac{(-i)^n}{n!}\int_0^\beta d\tau'_1 ... \int_0^\beta d\tau'_n Tr\left[\mathcal{T}[a_{I,k}(\tau)a^\dagger_{I,k}(0)V_I(\tau'_1)...V_I(\tau'_n)]\right] \tag{59}$$

From diagrammatic analysis, we will observe that D_n are all represented by disconnected diagrams, and

$$C_0+\sum_n C_n = \left(C_0+\sum_n C_{n,,connected}\right)\times D_n \tag{60}$$

From (55), we will have

$$-\mathcal{G}(k,\tau) = -\mathcal{G}^0(k,\tau)+\sum_{n=1}^{\infty} C_{n,connected} \tag{61}$$

See figure (1)

1.6 Self-energy

From diagram in figure (10) one can write the interacting Green's function in term of perturbation series as

$$G = G^0+G^0\Sigma G^0+G^0\Sigma G^0\Sigma G^0+... = G^0+G^0\Sigma G \tag{62}$$

$$(1-G^0\Sigma)G = G^0 \rightarrow G^{-1} = (G^0)^{-1}-\Sigma \tag{63}$$

Since $(G^0)^{-1} = \omega-\xi_k+i\eta$, so that

$$G(k,\omega) = \frac{1}{\omega-\xi_k-\Sigma(k,\omega)+i\eta} \tag{64}$$

See figure (2) for diagrammatic representation of σ.

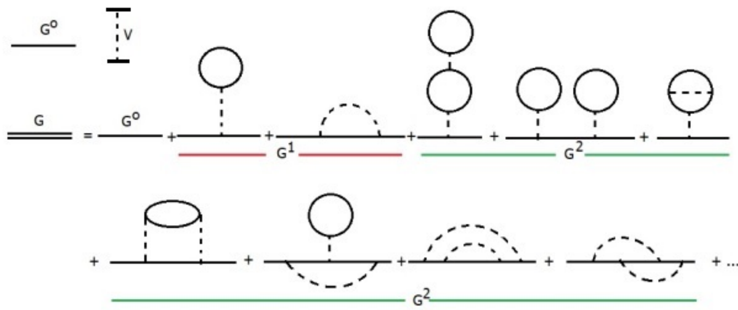

Figure 1: Diagrammatic representation of interacting Green's function.

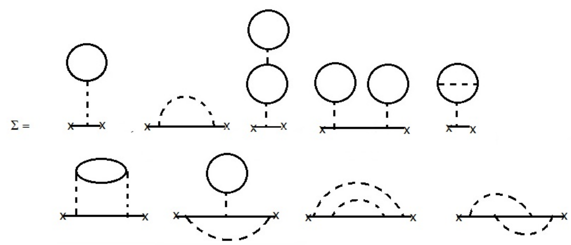

Figure 2: Self-energy diagrams.

1.7 Vertex

See figure (3)

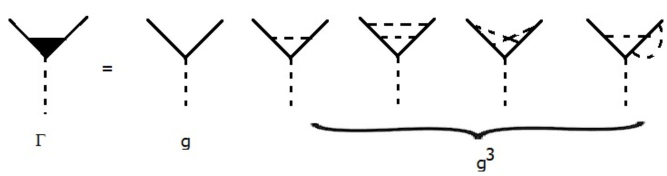

Figure 3: Vertex diagrams.

1.8 Screened interaction

See figure (4)

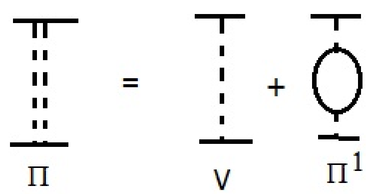

Figure 4: Screened interaction diagrams.