Chap 7 Finite-temperature Green function

Ming-Che Chang

Department of Physics, National Taiwan Normal University, Taipei, Taiwan

(Dated: January 12, 2018)

I. INTRODUCTION

At $T=0$, to get the expectation value of an observable in the ground state, one only needs to take the quantum average,

$$\langle A\rangle = \langle \Psi_0|A|\Psi_0\rangle. \tag{1}$$

At $T\neq 0$, both quantum average and thermal average are required,

$$\langle A\rangle_T = \sum_n \frac{e^{-\beta E_n}}{Z}\langle \Psi_n|A|\Psi_n\rangle, \tag{2}$$

in which $\beta = 1/k_BT$, Z is the partition function, and Ψ_n is the manybody eigenstates.

If the number of particles is not conserved, then we need to use the **grand canonical ensemble**, and

$$\langle A\rangle_{T,\mu} = \sum_{N=0}^{\infty}\sum_n \frac{e^{-\beta(E_n^N-\mu N)}}{\mathcal{Z}}\langle \Psi_n^N|A|\Psi_n^N\rangle, \tag{3}$$

where

$$\mathcal{Z} = \sum_{N,n} e^{-\beta(E_n^N-\mu N)} \equiv e^{-\beta\Omega}, \tag{4}$$

in which Ω is known as the **grand potential**. Define the **grand canonical Hamiltonian** and the **density operator** as,

$$\hat{K} = \hat{H}-\mu\hat{N}, \tag{5}$$

$$\hat{\rho}_G = \frac{1}{\mathcal{Z}}e^{-\beta\hat{K}} = e^{\beta(\Omega-\hat{K})}, \tag{6}$$

then (neglect ˆ from now on)

$$\mathcal{Z} = \mathrm{Tr}\; e^{-\beta K} \quad (\text{trace over } |\Psi_n^N\rangle), \tag{7}$$

$$\text{and } \langle A\rangle_{T,\mu} = \mathrm{Tr}\left[e^{\beta(\Omega-K)}A\right] = \mathrm{Tr}(\rho_G A). \tag{8}$$

II. GREEN FUNCTION

The finite-temperature Green function is defined as,

$$\begin{aligned} G_{\alpha\beta}(t,t') &= -i\sum_{N,n}\frac{e^{-\beta(E_n^N-\mu N)}}{\mathcal{Z}}\langle \Psi_n^N|Ta_\alpha(t)a_\beta^\dagger(t')|\Psi_n^N\rangle \\ &= -i\mathrm{Tr}\left[e^{\beta(\Omega-K)}Ta_\alpha(t)a_\beta^\dagger(t')\right], \end{aligned} \tag{9}$$

where

$$a_\alpha(t) = e^{iKt/\hbar}a_\alpha e^{-iKt/\hbar}, \tag{10}$$

$$a_\alpha^\dagger(t) = e^{iKt/\hbar}a_\alpha^\dagger e^{-iKt/\hbar}. \tag{11}$$

There are two types of exponential in the trace, $\rho_G = e^{-\beta K}/\mathcal{Z}$ and $U(t)=e^{-iKt/\hbar}$. They satisfy

$$\frac{\partial \rho_G}{\partial\beta} = -K\rho_G, \tag{12}$$

$$\text{and } \frac{i}{\hbar}\frac{\partial U}{\partial t} = KU. \tag{13}$$

These two equation are formally the same if we identify

$$t=-i\hbar\tau, \text{ or } \tau = it/\hbar \in R. \tag{14}$$

Thus, define the **Matsubara-Green function** as,

$$G_{\alpha\beta}(\tau,\tau') = -\mathrm{Tr}\left[e^{\beta(\Omega-K)}T_\tau a_\alpha(\tau)\bar{a}_\beta(\tau')\right], \tag{15}$$

in which

$$a_\alpha(\tau) \equiv e^{K\tau}a_\alpha e^{-K\tau}, \tag{16}$$

$$\bar{a}_\alpha(\tau) \equiv e^{K\tau}a_\alpha^\dagger e^{-K\tau}. \tag{17}$$

These two operators are *not* hermitian conjugate to each other when τ is real. From now on we set $\hbar=1$.

A. Basic property

The Matsubara-Green function $G_{\alpha\beta}(\tau,\tau')$ has the following properties:
1. $G_{\alpha\beta}(\tau,\tau') = G_{\alpha\beta}(\tau-\tau')$.
Pf: For $\tau>\tau'$,

$$\begin{aligned} G_{\alpha\beta}(\tau,\tau') &= -e^{\beta\Omega}\mathrm{Tr}\left[e^{-\beta K}e^{K\tau}a_\alpha e^{-K(\tau-\tau')}a_\beta^\dagger e^{-K\tau'}\right] \\ &= -e^{\beta\Omega}\mathrm{Tr}\left[e^{-\beta K}e^{K(\tau-\tau')}a_\alpha e^{-K(\tau-\tau')}a_\beta^\dagger\right] \\ &= G_{\alpha\beta}(\tau-\tau'). \end{aligned} \tag{18}$$

The proof for $\tau'>\tau$ is similar.
2. $G_{\alpha\beta}(\tau)$ is discontinuous across $\tau=0$.
Pf: We consider the cases for bosons and fermions simultaneously,

$$\begin{aligned} G_{\alpha\beta}(0^+)-G_{\alpha\beta}(0^-) &= -\mathrm{Tr}\; e^{\beta(\Omega-K)}\underbrace{\left(a_\alpha a_\beta^\dagger \mp a_\beta^\dagger a_\alpha\right)}_{\delta_{\alpha\beta}} \\ &= -\delta_{\alpha\beta}. \end{aligned} \tag{19}$$

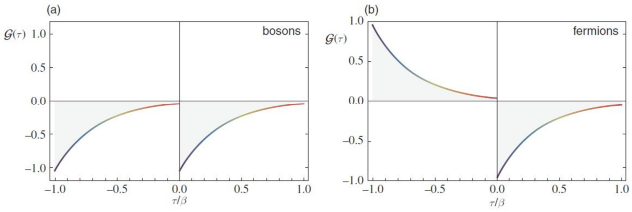


FIG. 1 Matsubara Green function $G_\alpha(\tau)$ for (a) bosons, and (b) fermions. Fig from Coleman's note.

The upper sign is for boson, and the lower sign is for fermion. 3. $G_{\alpha\beta}(\tau)$ converges only if $-\beta < \tau < \beta$.
Pf: If $\tau > 0$, then

$$G_{\alpha\beta}(\tau) = -e^{\beta\Omega}\mathrm{Tr}\left[e^{K(\tau-\beta)}a_\alpha e^{-K\tau}a_\beta^\dagger(0)\right]. \tag{20}$$

Because the energy eigenvalues would approach $+\infty$ (but not $-\infty$), the exponential factor $e^{-K\tau}$ converges, and $e^{K(\tau-\beta)}$ also converges when $0 < \tau < \beta$.
Similarly, if $\tau < 0$, then the exponential factor $e^{K\tau}$ converges, and $e^{-K(\beta+\tau)}$ also converges only when $-\beta < \tau < 0$.
4. Periodicity:

$$\begin{aligned} G_{\alpha\beta}(\tau) &= \pm G_{\alpha\beta}(\tau+\beta) \text{ for } \tau < 0, & (21)\\ G_{\alpha\beta}(\tau) &= \pm G_{\alpha\beta}(\tau-\beta) \text{ for } \tau > 0. & (22)\end{aligned}$$

Pf: For $\tau < 0$,

$$\begin{aligned} G_{\alpha\beta}(\tau+\beta) &= -e^{\beta\Omega}\mathrm{Tr}\left[e^{-\beta K}e^{(\tau+\beta)K}a_\alpha e^{-(\tau+\beta)K}a_\beta^\dagger\right] \\ &= -e^{\beta\Omega}\mathrm{Tr}\left[e^{\tau K}a_\alpha e^{-\tau K}e^{-\beta K}a_\beta^\dagger\right] \\ &= -e^{\beta\Omega}\mathrm{Tr}\,[e^{-\beta K}\underbrace{a_\beta^\dagger a_\alpha(\tau)}_{=\pm T_\tau a_\alpha(\tau)a_\beta^\dagger}] \\ &= \pm G_{\alpha\beta}(\tau). & (23)\end{aligned}$$

The proof for $\tau > 0$ is similar.
The result of these four properties is summarized in Fig. 1.

B. Fourier transformation

Since $G_{\alpha\beta}(\tau)$ is defined within the interval $[-\beta,\beta]$, it can be expanded as,

$$G_{\alpha\beta}(\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\pi n\tau/\beta}G_{\alpha\beta}(n). \tag{24}$$

Its inverse transformation is,

$$\begin{aligned} &G_{\alpha\beta}(n) \\ =\ & \frac{1}{2}\int_{-\beta}^{\beta} d\tau e^{i\pi n\tau/\beta}G_{\alpha\beta}(\tau) \\ =\ & \frac{1}{2}\int_{-\beta}^{0} d\tau e^{i\pi n\tau/\beta}\underbrace{G_{\alpha\beta}(\tau)}_{\pm G_{\alpha\beta}(\tau+\beta)} + \frac{1}{2}\int_{0}^{\beta} d\tau e^{i\pi n\tau/\beta}G_{\alpha\beta}(\tau) \\ =\ & \frac{e^{-i\pi n}}{2}\int_0^\beta d\tau' e^{i\pi n\tau'/\beta}[\pm G_{\alpha\beta}(\tau')] + \text{2nd term above} \\ =\ & \int_0^\beta d\tau e^{i\pi n\tau/\beta}G_{\alpha\beta}(\tau), & (25)\end{aligned}$$

in which n is even for boson, odd for fermion. That is,

$$G_{\alpha\beta}(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n\tau}G_{\alpha\beta}(\tau), \tag{26}$$

$$\begin{cases} \omega_n = 2n\frac{\pi}{\beta} & \text{for bosons,} \\ \omega_n = (2n+1)\frac{\pi}{\beta} & \text{for fermions.} \end{cases} \tag{27}$$

The frequency ω_n is known as the **Matsubara frequency**.

A brief summary:
To move from $T = 0$ to $T \neq 0$, the following substitution is required:

$$\begin{aligned} &1.\ it \to \tau, & (28)\\ &2.\ \omega \to i\omega_m, & (29)\\ &3.\ \int_{-\infty}^{\infty} dt e^{i\omega t} \to \int_0^\beta d\tau e^{i\omega_m\tau}, & (30)\\ &4.\ \int d\omega e^{-i\omega t} \to \frac{1}{\beta}\sum_{i\omega_m} e^{-i\omega_m\tau}. & (31)\end{aligned}$$

C. Spectral representation

Consider the following ground-state average at $T = 0$,

$$C_{AB}^R(t) = -i\theta(t)\langle[A(t),B(0)]_\mp\rangle_0, \tag{32}$$

where A, B are a_α and/or $a_\alpha^\dagger$. If $(A,B) = (a_\alpha, a_\beta^\dagger)$, then $C_{AB}^R(t)$ is the retarded Green function $G_{\alpha\beta}^R$. Recall that (Chap 6),

$$\begin{aligned} C_{AB}^R(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t}C_{AB}^R(t) & (33)\\ &= \sum_n\left(\frac{A_{0n}B_{n0}}{\omega-\omega_{n0}+i\eta} \mp \frac{B_{0n}A_{n0}}{\omega+\omega_{n0}+i\eta}\right), & (34)\end{aligned}$$

in which $\omega_{nm} \equiv \omega_n - \omega_m$. When $T \neq 0$, but still with real time and canonical ensemble,

$$\begin{aligned} &C_{AB}^R(\omega) \\ =\ & \sum_{mn}P_m\left(\frac{A_{mn}B_{nm}}{\omega-\omega_{nm}+i\eta} \mp \frac{B_{mn}A_{nm}}{\omega+\omega_{nm}+i\eta}\right), & (35)\\ =\ & \sum_{mn}(P_m \mp P_n)\frac{A_{mn}B_{nm}}{\omega-\omega_{nm}+i\eta},\ \ P_n = \frac{e^{-\beta E_n}}{Z}. & (36)\end{aligned}$$

Now with imaginary time (still in canonical ensemble), for $\tau > 0$, define

$$\begin{aligned} C_{AB}(\tau) &= -\langle T_\tau A(\tau) B(0)\rangle & (37)\\ &= -\frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H} e^{\tau H} A e^{-\tau H} B\right) & (38)\\ &= -\frac{1}{Z}\sum_{mn} e^{-\beta E_m} e^{-\tau(E_n-E_m)} A_{mn} B_{nm}. & (39)\end{aligned}$$

It follows that,

$$\begin{aligned} C_{AB}(i\omega_\ell) &= \int_0^\beta d\tau e^{i\omega_\ell \tau}\left(-\sum_{mn} P_m e^{-\tau(E_n-E_m)} A_{mn} B_{nm}\right)\\ &= \sum_{mn}(P_m \mp P_n)\frac{A_{mn}B_{nm}}{i\omega_\ell - \omega_{nm}}. & (40)\end{aligned}$$

Comparing Eq. (36) with Eq. (40), we have

$$C^R_{AB}(\omega) = C_{AB}(i\omega_\ell \to \omega + i\eta). \quad (41)$$

The advanced function can be obtained in a similar way with the substitution $i\omega_\ell \to \omega - i\eta$. This remains valid for grand canonical ensemble. One only needs to replace

$$\begin{aligned} E_n &\to K_n = E_n - \mu N, & (42)\\ \text{and } \sum_n &\to \sum_{N,n}, \quad Z \to \mathcal{Z}. & (43)\end{aligned}$$

Note (important): The analytic continuation $i\omega_\ell \to \omega \pm i\eta$ *cannot* be applied *before* doing the τ-integral. See p. 263 (and p.297) of Ref. 3.

In the spectral representation, the Matsubara-Green function for fermions can be written as,

$$\begin{aligned} G_{\alpha\beta}(i\omega_\ell) &= \sum_{mn}(P_m + P_n)\frac{(a_\alpha)_{mn}(a^\dagger_\beta)_{nm}}{i\omega_\ell - \omega_{nm}} & (44)\\ &= \int \frac{d\omega}{2\pi}\frac{A_{\alpha\beta}(\omega)}{i\omega_\ell - \omega}, & (45)\end{aligned}$$

where

$$\begin{aligned} A_{\alpha\beta}(\omega) &\equiv 2\pi\sum_{mn}(P_m + P_n)(a_\alpha)_{mn}(a^\dagger_\beta)_{nm}\delta(\omega - \omega_{nm})\\ \text{also } &= -2\,\mathrm{Im}\, G_{\alpha\beta}(i\omega_\ell \to \omega + i\eta). & (46)\end{aligned}$$

III. NON-INTERACTING SYSTEM

Consider non-interacting bosons/fermions with the grand canonical Hamiltonian,

$$K_0 = H_0 - \mu N = \sum_\alpha (\varepsilon_\alpha - \mu) a^\dagger_\alpha a_\alpha. \quad (47)$$

In the Heisenberg picture, $a_\alpha(t) = e^{iH_0 t} a_\alpha e^{-iH_0 t}$. Also,

$$\begin{aligned} e^{-\mu N} a_\alpha e^{\mu N} &= e^{\mu} a_\alpha, & (48)\\ e^{-\mu N} a^\dagger_\alpha e^{\mu N} &= e^{-\mu} a^\dagger_\alpha. & (49)\end{aligned}$$

Since $[H_0, N] = 0$, we have

$$\begin{aligned} a_\alpha(\tau) &= e^{K_0\tau} a_\alpha e^{-K_0\tau} = e^{-\tilde\varepsilon_\alpha \tau} a_\alpha, & (50)\\ \bar a_\alpha(\tau) &= e^{K_0\tau} a^\dagger_\alpha e^{-K_0\tau} = e^{\tilde\varepsilon_\alpha \tau} a^\dagger_\alpha, & (51)\end{aligned}$$

where $\tilde\varepsilon_\alpha \equiv \varepsilon_\alpha - \mu$.

One can show that,

$$\begin{aligned} \langle a^\dagger_\alpha a_\beta\rangle_0 &= \frac{\delta_{\alpha\beta}}{e^{\beta\tilde\varepsilon_\alpha} \mp 1} = n_\alpha \delta_{\alpha\beta}, & (52)\\ \text{where } n_\alpha &\equiv \frac{1}{e^{\beta\tilde\varepsilon_\alpha} \mp 1}.\end{aligned}$$

Pf: Ref: p. 224 of Kubo, Statistical Physics II.

$$\begin{aligned} \langle a^\dagger_\alpha a_\beta\rangle_0 &= \mathrm{Tr}\left(\frac{e^{-\beta K_0}}{\mathcal{Z}} a^\dagger_\alpha a_\beta\right) & (53)\\ &= \frac{1}{\mathcal{Z}}\mathrm{Tr}\left(1 a_\beta e^{-\beta K_0} a^\dagger_\alpha\right) & (54)\\ &= e^{-\beta\tilde\varepsilon_\alpha}\langle a_\beta a^\dagger_\alpha\rangle_0, & (55)\end{aligned}$$

where we have inserted $e^{-\beta K_0} e^{\beta K_0}$ at the location "1". From the (anti-) commutation relation, one has

$$\mp\langle a^\dagger_\alpha a_\beta\rangle_0 = \delta_{\alpha\beta} - \langle a_\beta a^\dagger_\alpha\rangle_0, \quad (56)$$

and Eq. (52) follows.

With time dependence, we have

$$\langle a_\alpha(\tau)\bar a_\beta(\tau')\rangle_0 = e^{-\tilde\varepsilon_\alpha(\tau-\tau')}\langle a_\alpha a^\dagger_\alpha\rangle_0 \delta_{\alpha\beta}. \quad (57)$$

Therefore,

$$\begin{aligned} & G^0_{\alpha\beta}(\tau-\tau')\\ =& -\langle T_\tau a_\alpha(\tau)\bar a_\beta(\tau')\rangle_0\\ =& -\theta(\tau-\tau')\langle a_\alpha(\tau)\bar a_\beta(\tau')\rangle_0 \mp \theta(\tau'-\tau)\langle \bar a_\beta(\tau') a_\alpha(\tau)\rangle_0\\ =& -\delta_{\alpha\beta}\left[\theta(\tau-\tau')(1 \pm n_\alpha) \pm \theta(\tau'-\tau) n_\alpha\right] e^{-\tilde\varepsilon_\alpha(\tau-\tau')}. \quad (58)\end{aligned}$$

See Fig. 1 for plots of the non-interacting Matsubara-Green functions. Its Fourier transformation gives,

$$\begin{aligned} G^0_\alpha(i\omega_n) &= \int_0^\beta d\tau e^{i\omega_n\tau} G^0_\alpha(\tau)\\ &= -(1 \pm n_\alpha)\int_0^\beta d\tau e^{(i\omega_n - \tilde\varepsilon_\alpha)\tau}\\ &= \frac{1}{i\omega_n - \tilde\varepsilon_\alpha}. & (59)\end{aligned}$$

Note that $G^0_\alpha(i\omega_n \to \omega + i\eta)$ gives the non-interacting retarded Green function.

Now we transform the Matsubara-Green function back to the time domain,

$$G^0_\alpha(\tau) = \frac{1}{\beta}\sum_{i\omega_n}\underbrace{e^{-i\omega_n\tau} G^0_\alpha(i\omega_n)}_{\equiv g(i\omega_n)}, \quad (60)$$

where $\omega_n = 2n\pi/\beta$ for bosons, or $(2n+1)\pi/\beta$ for fermions. A trick can be used to evaluate the summation:

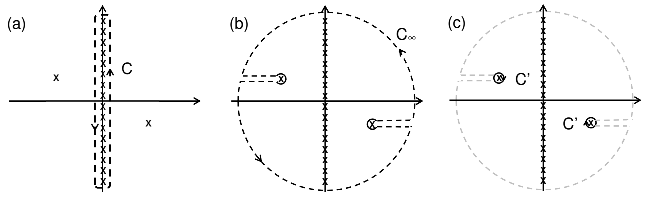


FIG. 2 (a) Poles at $i\omega_n$ and the encircling path. (b) An inflated path of integration, avoiding the other poles. (c) Since the large circle and the opposing horizontal paths in (b) make no contribution, only the small circles around other poles are left.

First, note that the Matsubara frequencies $i\omega_n$ are poles of the distribution functions,

$$n(z) = \frac{1}{e^{\beta z}-1} \text{ for bosons,} \tag{61}$$

$$\text{or} = \frac{1}{e^{\beta z}+1} \text{ for fermions.} \tag{62}$$

Therefore,

$$\frac{1}{2\pi i}\oint_c n(z)g(z)dz = \pm\frac{1}{\beta}\sum_{i\omega_n} g(i\omega_n). \tag{63}$$

Pf: Because of the **Cauchy residue theorem**,

$$\frac{1}{2\pi i}\oint_c n(z)g(z)dz = \sum_\ell \text{Res } [n(z_\ell)]g(z_\ell), \tag{64}$$

in which C is the path in Fig. 2(a). Near a pole,

$$\frac{1}{e^{\beta z}\mp 1} = \frac{1}{e^{\beta i\omega_n}e^{\beta(z-i\omega_n)}\mp 1} \tag{65}$$

$$\simeq \frac{1}{\pm[1+\beta(z-i\omega_n)]\mp 1} \tag{66}$$

$$= \pm\frac{1/\beta}{z-i\omega_n}. \tag{67}$$

Therefore,

$$\text{Res } n(i\omega_n) = \pm\frac{1}{\beta}, \tag{68}$$

and Eq. (63) follows.

Second, we now inflate the contour C to a large circle, but avoid crossing the poles of $g(z)$ (see Fig. 2(b)). If $n(z)g(z)$ decays faster than $1/z$, then the integral around the circle at infinity is zero. Therefore, only the integration around the poles of $g(z)$ survive (see Fig. 2(c)),

$$\oint_c dz = \oint_{c_\infty} dz + \underbrace{\oint_{c'}}_{\text{clockwise}} dz \tag{69}$$

$$= 0 - \oint_{\bar{c}'} dz, \quad (\bar{c}' \text{ is counter}-\text{clockwise}). \tag{70}$$

Apply the Cauchy residue theorem to the second integral, it follows that (cf: Eq. (64)),

$$\pm\frac{1}{\beta}\sum_{i\omega_n} g(i\omega_n) = -\sum_\ell n(z_\ell)\text{Res } g(z_\ell), \tag{71}$$

where z_ℓ are the poles of $g(z)$.

Now, choose

$$g(z) = e^{-\tau z}G^0_\alpha(z) = \frac{e^{-\tau z}}{z-\tilde{\varepsilon}_\alpha}, \tag{72}$$

which has a simple pole at $\tilde{\varepsilon}_\alpha$, and Res $g(z_\ell) = e^{-\tau\tilde{\varepsilon}_\alpha}$. Also, note that

$$n(z)g(z) \simeq e^{-\beta z}e^{-\tau z}/z \text{ for Re}(z) \gg 0, \tag{73}$$

$$\simeq \mp e^{-\tau z}/z \text{ for Re}(z) \ll 0. \tag{74}$$

Both cases lead to converged result if $-\beta < \tau < 0$. Therefore, from Eqs. (60) and (71), we have

$$G^0_\alpha(\tau<0) = \frac{1}{\beta}\sum_{i\omega_n} g(i\omega_n) \tag{75}$$

$$= \mp\frac{1}{e^{\beta\tilde{\varepsilon}_\alpha}\mp 1}e^{-\tilde{\varepsilon}_\alpha\tau}$$

$$= \mp n(\tilde{\varepsilon}_\alpha)e^{-\tilde{\varepsilon}_\alpha\tau}. \tag{76}$$

What if $\tau > 0$? In this range, we need to choose

$$n(-z) = \frac{1}{e^{-\beta z}\mp 1}, \tag{77}$$

then

$$n(-z)g(z) \simeq \mp e^{-\tau z}/z \text{ for Re}(z) \gg 0, \tag{78}$$

$$\simeq e^{\beta z}e^{-\tau z}/z \text{ for Re}(z) \ll 0. \tag{79}$$

Both cases lead to converged result if $0 < \tau < \beta$. Therefore,

$$G^0_\alpha(\tau>0) = \pm\frac{1}{e^{-\beta\tilde{\varepsilon}_\alpha}\mp 1}e^{-\tilde{\varepsilon}_\alpha\tau}$$

$$= \pm n(-\tilde{\varepsilon}_\alpha)e^{-\tilde{\varepsilon}_\alpha\tau}. \tag{80}$$

Since

$$1\pm n(\tilde{\varepsilon}_\alpha) = \mp n(-\tilde{\varepsilon}_\alpha), \tag{81}$$

combining Eqs. (76) and (80), we are back to Eq. (58).

For reference, for bosons/fermions, one has

$$n(\tilde{\varepsilon}_\alpha)[1\pm n(\tilde{\varepsilon}_\alpha)] = -\frac{1}{\beta}\frac{dn}{d\tilde{\varepsilon}_\alpha}. \tag{82}$$

It follows that, for *fermions*,

$$\lim_{T\to 0}\beta n(1-n) = \delta(\tilde{\varepsilon}_\alpha). \tag{83}$$

IV. INTERACTING SYSTEM

For an interacting fermion system,

$$H = H_0 + H', \quad (84)$$
$$\text{or } K = K_0 + H'. \quad (85)$$

$$G_{\alpha\beta}(\tau,\tau') = -\langle T_\tau a_\alpha(\tau)\bar{a}_\beta(\tau')\rangle \quad (86)$$
$$= -\frac{\mathrm{Tr}\left[e^{-\beta K}T_\tau a_\alpha(\tau)\bar{a}_\beta(\tau')\right]}{\mathrm{Tr}\,(e^{-\beta K})}, \quad (87)$$

in which $a_\alpha(\tau) = e^{K\tau}a_\alpha e^{-K\tau}$, and one traces over *exact* manybody energy eigenstates $|\Psi_n^N\rangle$. Similar to the $T=0$ case in the preceding chapter, we treat the interaction as a perturbation and trace over non-interacting states $|\Phi_n^N\rangle$. Note that here the adiabatic assumption is *not* required.

First, write

$$e^{-K\tau} = e^{-K_0\tau}U_I(\tau,0), \quad (88)$$

where $U_I(\tau,\tau') = e^{K_0\tau}e^{-K(\tau-\tau')}e^{-K_0\tau'}$. Then,

$$\frac{\partial U_I(\tau)}{\partial\tau} = e^{K_0\tau}(K_0-K)e^{-K_0\tau}U_I(\tau,0)$$
$$= -H_I'(\tau)U_I(\tau,0). \quad (89)$$

It follows that,

$$U_I(\tau,0) = \sum_n \frac{(-1)^n}{n!}\int_0^\tau d\tau_1\cdots d\tau_n T_\tau[H_I'(\tau_1)\cdots H_I'(\tau_n)]$$
$$= T_\tau e^{-\int_0^\tau d\tau' H_I'(\tau')}. \quad (90)$$

Since $a_{I\alpha}(\tau) = e^{K_0\tau}a_\alpha e^{-K_0\tau}$, we have

$$a_\alpha(\tau) = \underbrace{e^{K\tau}e^{-K_0}}_{U_I(0,\tau)}a_{I\alpha}(\tau)\underbrace{e^{K_0\tau}e^{-K\tau}}_{U_I(\tau,0)}, \quad (91)$$
$$\bar{a}_\beta(\tau') = U_I(0,\tau')\bar{a}_{I\beta}(\tau')U_I(\tau',0). \quad (92)$$

Also, write

$$e^{-\beta K} = e^{-\beta K_0}U_I(\beta,0), \quad (93)$$

then for $\tau > \tau'$,

$$G_{\alpha\beta}(\tau,\tau') \quad (94)$$
$$= -\frac{\mathrm{Tr}\left[e^{-\beta K_0}U_I(\beta,\tau)a_{I\alpha}(\tau)U_I(\tau,\tau')\bar{a}_{I\beta}(\tau')U_I(\tau',0)\right]}{\mathrm{Tr}\left[e^{-\beta K_0}U_I(\beta,0)\right]}.$$

The case for $\tau < \tau'$ works similarly. Thus, the Matsubara-Green function can be written as,

$$G_{\alpha\beta}(\tau,\tau') = -\frac{\langle T_\tau U_I(\beta,0)a_{I\alpha}(\tau)\bar{a}_{I\beta}(\tau')\rangle_0}{\langle U_I(\beta,0)\rangle_0} \quad (95)$$
$$= -\frac{\langle T_\tau e^{-\int_0^\beta d\tau'' H_I'(\tau'')}a_{I\alpha}(\tau)\bar{a}_{I\beta}(\tau')\rangle_0}{\langle T_\tau\ e^{-\int_0^\beta d\tau' H_I'(\tau')}\rangle_0}. \quad (96)$$

The subscript "0" means that we use $e^{-\beta K_0}$ for thermal average and trace over non-interacting eigenstates $|\Phi_n^N\rangle$. This is the finite-temperature generalization of the Gell-mann and Low theorem. To calculate it, we need to expand the exponential with the interaction. Again the Wick theorem would be of great help for our calculations.

A. Wick theorem

Recall that for $T=0$, the Wick theorem (1950) is about moving a_α to the right, and taking advantage of $a_\alpha|\Phi_0\rangle = 0$. It is an operator identity, and the ground-state average of the operator product is eventually left with fully contracted terms.

In comparison, the Wick theorem for $T \neq 0$ (1955) is *not* about moving a_α to the right, since $a_\alpha|\Phi_n\rangle \neq 0$ for excited states. Also, it is *not* an operator identity, since ensemble average is required, and the thermal factor $e^{-\beta K_0}$ is essential for this theorem. However, the algebraic forms of this two theorems are quite similar, and the Matsubara-Green function would also be decomposed as fully contracted terms.

First, recall that

$$\langle A\rangle_0 = \mathrm{Tr}(\rho_0 A),\ \rho_0 = \frac{e^{-\beta K_0}}{\mathrm{Tr}\,(e^{-\beta K_0})} = e^{\beta\Omega-\beta K_0}. \quad (97)$$

Second, the **contraction** between two operators is defined as,

$$\overbrace{AB} = \langle T_\tau AB\rangle_0 = \mathrm{Tr}\{\rho_0 T_\tau(AB)\}. \quad (98)$$

For example,

$$\overbrace{a_\alpha a_\beta} = 0, \quad (99)$$
$$\overbrace{a_\alpha^\dagger a_\beta^\dagger} = 0, \quad (100)$$
$$\overbrace{a_\alpha^\dagger a_\beta} = \langle a_\alpha^\dagger a_\beta\rangle = \frac{\delta_{\alpha\beta}}{e^{\beta\tilde{\varepsilon}_k}\mp 1} = n_\alpha\delta_{\alpha\beta}, \quad (101)$$
$$\overbrace{a_\alpha a_\beta^\dagger} = \langle a_\alpha a_\beta^\dagger\rangle = \frac{\delta_{\alpha\beta}}{1\mp e^{-\beta\tilde{\varepsilon}_k}} = (1\pm n_\alpha)\delta_{\alpha\beta}, \quad (102)$$
$$\overbrace{a_\alpha(\tau)\bar{a}_\beta(\tau')} = -G_{\alpha\beta}^0(\tau,\tau'). \quad (103)$$

The Wick theorem at finite temperature goes as,

$$\langle T_\tau ABC\cdots XYZ\rangle_0 \quad (104)$$
$$= \langle T_\tau \overbrace{AB}C\cdots XYZ\rangle_0 + \langle T_\tau \overbrace{ABC}\cdots XYZ\rangle_0 + \cdots,$$

where $A, B, \cdots$ are creation or annihilation operators. The contracted terms can be moved out of the brackets. One then keeps contracting the operators till everyone is paired. A proof of this theorem can be found in, e.g., p. 679 of Ref. 1.

It's clear that, further derivation just duplicate the analysis in the $T=0$ theory. For example, the $T\neq 0$ theory also has the **linked cluster theorem** and the **Dyson equation** (see Chap 6).

V. GREEN FUNCTION IN MOMENTUM SPACE

Consider

$$K = \sum_{k\alpha}(\varepsilon_{k\alpha}-\mu)a_{k\alpha}^\dagger a_{k\alpha} + V_{ee}, \quad (105)$$

the Matsubara-Green function at the zeroth order is,

$$G^0_{\alpha\beta}(\mathbf{k}, i\omega_n) = \frac{1}{V_0}\sum_k \int_0^\beta d\tau e^{i\omega_n\tau} e^{-i\mathbf{k}\cdot\mathbf{r}} G^0_{\alpha\beta}(\mathbf{r},\tau)$$
$$= \delta_{\alpha\beta}\frac{1}{i\omega_n - \tilde{\varepsilon}_{k\alpha}}. \quad (106)$$

To the first order,

$$G_{\alpha\beta}(\mathbf{k}, i\omega_n) = G^0_{\alpha\beta}(\mathbf{k}, i\omega_n) \quad (107)$$
$$- \int_0^\beta d\tau e^{i\omega_n(\tau-\tau')}(-1)\int d\tau_1 \langle T_\tau V_{ee}(\tau_1) a_{k\alpha}(\tau)\bar{a}_{k\beta}(\tau')\rangle_{0,c},$$

where

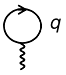
$$V_{ee}(\tau) = \frac{1}{2V_0}\sum_{k_1k_2q} V^{(2)}_{\gamma_1\gamma_2\gamma_2\gamma_1}(\mathbf{q})\bar{a}_{k_1+q,\gamma_1}\bar{a}_{k_2-q,\gamma_2}a_{k_2\gamma_2}a_{k_1\gamma_1}. \quad (108)$$

The operators are all at the same time τ. To contract operators with the same time, use

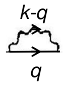
$$\langle \bar{a}_\alpha a_\beta\rangle = -\langle T_\tau a_\beta a^\dagger_\alpha(0^+)\rangle$$
$$= G^0_{\beta\alpha}(0^-)$$
$$= \frac{1}{\beta}\sum_n e^{i\omega_n\eta}G_{\beta\alpha}(i\omega_n), \quad \eta = 0^+. \quad (109)$$

That is, when $G^0_{\alpha\beta}$ connects to the same wavy line, the factor $e^{i\omega_n\eta}$ needs be inserted.

Using the Wick theorem, and following the same procedure as the $T=0$ theory, one would get the Hartree-Fock self-energy below (see Chap 6, assuming $\varepsilon_{k\alpha} = \varepsilon_k$ is spin-independent),



$$= -2\int\frac{d^3q}{(2\pi)^3}\underbrace{\frac{1}{\beta}\sum_n G^0(\mathbf{q}, i\omega_n)e^{i\omega_n\eta}}_{G^0(\mathbf{q},0^-)}[-V(0)], \quad (110)$$



$$= \int\frac{d^3q}{(2\pi)^3}\frac{1}{\beta}\sum_n G^0(\mathbf{q}, i\omega_n)e^{i\omega_n\eta}[-V(\mathbf{k}-\mathbf{q})] \quad (111)$$

The Matsubara-Green function is spin-independent, and the subscript is omitted (see Eq. (58)),

$$G^0(\mathbf{q}, 0^-) = \frac{1}{e^{\beta\tilde{\varepsilon}_q}+1} = n_q. \quad (112)$$

It follows that,

$$\Sigma^H = 2\int\frac{d^3q}{(2\pi)^3}n_q V(0) = \frac{N}{V_0}V(0), \quad (113)$$
$$\Sigma^F = -\int\frac{d^3q}{(2\pi)^3}n_q V(\mathbf{k}-\mathbf{q}). \quad (114)$$

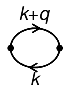
This is the same as the $T=0$ result in Chap 6, except that n_q can be a fraction of one.

At finite temperature, the Feynman rules for electron self-energy are:

1. At the n-th order, draw all topologically distinct connected diagrams with n wavy lines, $2n$ vertices, and $2n+1$ solid lines.
2. Each solid line is $G^0_{\alpha\beta}(k)$, $k \equiv (\mathbf{k}, i\omega_n)$. For a closed loop, or a segment linked by the same wavy line, alter it to $G^0_{\alpha\beta}(k)e^{i\omega_n\eta}$.
3. Each wavy line is $V^{(2)}_{\gamma'_1\gamma'_2\gamma_2\gamma_1}(q)$.
4. Associate each line with a 4-momentum, and the 4-momentum flow needs be conserved at each vertex.
5. Sum over internal degrees of freedom (4-momentum, spin ... etc), $(1/V_0)\sum_{k\alpha\cdots}$. The energy integral should be understood as the Matsubara-frequency sum.
6. Multiply the summation by $(-1)^n(-1)^F$, where n is the order (or half of the number of vertices), and F is the number of closed fermion loops. Note: for photon self-energy, n is one-half of the number of vertices (or the number of internal momenta).

This is essentially the same as the Feynman rules at zero temperature, except numerical factor in the last one.

For example, for the bubble diagram, we have



$$= (-1)^2 2\int\frac{d^3k}{(2\pi)^3}\frac{1}{\beta}\sum_m G^0(k)G^0(k+q)$$
$$\equiv \Pi^0(q), \quad (115)$$

in which $k = (\mathbf{k}, i\omega_m)$, $q = (\mathbf{q}, i\nu_n)$. Be aware that the ν_n from the photon propagator is *bosonic*, instead of fermionic. Now, for fermions, using

$$\frac{1}{\beta}\sum_{i\omega_n} f(i\omega_n) = \sum_\ell n(z_\ell)\text{Res } f(z_\ell), \quad (116)$$

we have

$$\frac{1}{\beta}\sum_m G^0G^0 = \frac{1}{\beta}\sum_m \frac{1}{i\omega_m - \tilde{\varepsilon}_k}\frac{1}{i\omega_m + i\nu_n - \tilde{\varepsilon}_{k+q}} \quad (117)$$
$$= \sum_\ell n(z_\ell)\text{Res}\left(\frac{1}{z-\tilde{\varepsilon}_k}\frac{1}{z+i\nu_n-\tilde{\varepsilon}_{k+q}}\right)$$
$$= \frac{1}{e^{\beta\tilde{\varepsilon}_k}+1}\frac{1}{i\nu_n+\tilde{\varepsilon}_k-\tilde{\varepsilon}_{k+q}}$$
$$+ \frac{1}{e^{\beta\tilde{\varepsilon}_{k+q}}+1}\frac{1}{-i\nu_n-\tilde{\varepsilon}_k+\tilde{\varepsilon}_{k+q}} \quad (118)$$
$$= \frac{n_k - n_{k+q}}{i\nu_n + \varepsilon_k - \varepsilon_{k+q}}. \quad (119)$$

Note that $e^{i\beta\nu_n} = 1$, since ν_n is bosonic. Thus,

$$\Pi^0(\mathbf{q}, i\nu_n) = 2\int\frac{d^3k}{(2\pi)^3}\frac{n_k - n_{k+q}}{i\nu_n + \varepsilon_k - \varepsilon_{k+q}}. \quad (120)$$

Again after the analytic continuation $i\nu_n \to \nu + i\eta$, it is the same as the Π^R_0 at $T=0$, except that now n_q can be a fraction of one.

One can consider the bubble diagram with dressed fermion lines,

$$\Pi(q) = 2\int\frac{d^3k}{(2\pi)^3}\frac{1}{\beta}\sum_m G(k)G(k+q), \quad (121)$$

in which

$$G(k) = \frac{1}{i\omega_n - \tilde{\varepsilon}_k - \Sigma(k)}. \qquad (122)$$

$\Sigma(k)$ is the proper self-energy due to, e.g., impurity scatterings (next Chap) or electron-electron interactions. Using the spectral representation in Eq. (45),

$$G(\mathbf{k}, i\omega_m) = \int \frac{d\omega}{2\pi} \frac{A_k(\omega)}{i\omega_m - \omega}, \qquad (123)$$

one has

$$\begin{aligned} &\frac{1}{\beta}\sum_m G(k)G(k+q) \\ =& \frac{1}{\beta}\sum_m \int_{-\infty}^{\infty} \frac{d\omega d\omega'}{(2\pi)^2} \frac{A_k(\omega)A_{k+q}(\omega')}{(i\omega_m - \omega)(i\omega_m + i\nu_n - \omega')} \qquad (124) \\ =& \int_{-\infty}^{\infty} \frac{d\omega d\omega'}{(2\pi)^2} A_k(\omega)A_{k+q}(\omega') \frac{n_k(\omega) - n_{k+q}(\omega' + i\nu_n)}{i\nu_n + \omega - \omega'} \qquad (125) \end{aligned}$$

The right-hand side can also be rewritten as,

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} n_k(\omega) \quad & [A_k(\omega)G(\mathbf{k}+\mathbf{q}, \omega + i\nu_n) \\ & + A_{k+q}(\omega)G(\mathbf{k}, \omega - i\nu_n)]. \qquad (126) \end{aligned}$$

Thus,

$$\begin{aligned} \Pi(q) &= 2\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int \frac{d^3k}{(2\pi)^3} n_k(\omega) \qquad (127) \\ &\times [A_k(\omega)G(\mathbf{k}+\mathbf{q}, \omega + i\nu_n) + A_{k+q}(\omega)G(\mathbf{k}, \omega - i\nu_n)]. \end{aligned}$$

Exercise:

1. Show that the real-time Green function at finite temperature (see Eq. (9)) satisfies,

$$\begin{aligned} G_{\alpha\beta}(t,t') &= \pm G_{\alpha\beta}(t + i\beta, t') \text{ for } t > t' \qquad (128) \\ &= \pm G_{\alpha\beta}(t - i\beta, t') \text{ for } t < t'. \qquad (129) \end{aligned}$$

2. Start from Eq. (60), using similar procedure that leads to Eq. (75) for $G^0_\alpha(\tau < 0)$, verify that the Matsubara-Green function $G^0_\alpha(\tau > 0)$ is given in Eq. (80).

3. (a) Show that the grand potential Ω for *non-interacting* bosons/fermions is

$$\Omega = \pm\frac{1}{\beta}\sum_{\alpha, i\omega_n} \ln(-i\omega_n + \tilde{\varepsilon}_\alpha)e^{i\omega_n\eta}. \qquad (130)$$

(b) Sum over the Matsubara frequencies, and show that

$$\Omega = \pm\frac{1}{\beta}\sum_\alpha \ln\left(1 \mp e^{-\beta\tilde{\varepsilon}_\alpha}\right). \qquad (131)$$

References

[1] Quantum Theory of the Electron Liquid, by Gabriele F. Giuliani and Giovanni Vignale, Cambridge University Press, 2005.

[2] Methods of Quantum Field Theory in Statistical Physics, by A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, Dover Publications, 1975.

[3] A.L. Fetter, J.D. Walecka, Quantum Theory of Many-Particle Systems, Dover Books, 2003.

[4] H. Bruss and K. Flensberg, *Many-body quantum theory in condensed matter physics*, Oxford University Press, 2004.