8.2. Boundary condition and connections between different Green's functions

8.2.1. Other correlation functions and the boundary condition

Define

$$G^{>}(1,2)=\frac{1}{i}\left\langle\psi(1)\,\psi^{\dagger}(2)\right\rangle \tag{8.31}$$

$$G^{<}(1,2)=\pm\frac{1}{i}\left\langle\psi^{\dagger}(2)\,\psi(1)\right\rangle \tag{8.32}$$

For statistical average, we have Boltzmann factor $e^{\beta H}$. For time-evolution, we have the evolution operator $e^{i H t}$. It seems that inverse temperature β is just the imaginary time. Let's try this idea by allowing time to be complex.

For $G^{>}$

$$G^{>}(1,2)=\frac{1}{i}\left\langle\psi(1)\,\psi^{\dagger}(2)\right\rangle=\frac{\operatorname{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\psi(r_1,\,t_1)\,\psi^{\dagger}(r_2,\,t_2)\right\}}{i\operatorname{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\right\}}=$$
$$\left(\operatorname{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\exp\left(i\,\hat{H}\,t_1\right)\psi(r_1)\exp\left(-i\,\hat{H}\,t_1\right)\exp\left(i\,\hat{H}\,t_2\right)\psi^{\dagger}(r_2)\exp\left(-i\,\hat{H}\,t_2\right)\right\}\right)\Big/\left(i\operatorname{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\right\}\right) \tag{8.33}$$

If we use eigenenergy states to compute the sum

$$G^{>}(1,2)=$$
$$\left(\sum_n\left\langle n\right|\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\exp\left(i\,\hat{H}\,t_1\right)\psi(r_1)\exp\left(-i\,\hat{H}\,t_1\right)\exp\left(i\,\hat{H}\,t_2\right)\psi^{\dagger}(r_2)\exp\left(-i\,\hat{H}\,t_2\right)\right\}\left|n\right\rangle\right)\Big/\left(i\operatorname{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\right\}\right)=$$
$$\exp[\beta\,\mu\,N]\left(\sum_n\exp[E_n(i\;t_1-\beta)]\left\langle n\left|\psi(r_1)\exp\left(-i\,\hat{H}\,t_1\right)\exp\left(i\,\hat{H}\,t_2\right)\psi^{\dagger}(r_2)\right|n\right\rangle\exp(-i\,E_n\,t_2)\right)\Big/\left(i\operatorname{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\right\}\right)=$$
$$\exp[\beta\,\mu\,N]\,\frac{\sum_n\exp[E_n(i\;t_1-i\,t_2-\beta)]\left\langle n\left|\psi(r_1)\exp\left(-i\,\hat{H}\,t_1\right)\exp\left(i\,\hat{H}\,t_2\right)\psi^{\dagger}(r_2)\right|n\right\rangle}{i\operatorname{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\right\}} \tag{8.34}$$

Because E_n has no upper bound, as $E_n\to+\infty$, to keep the factor $\exp[E_n(i\;t_1-i\,t_2-\beta)]$ converge, we need to have `Re (i t1 - i t2 - β) < 0`, In other words, $\operatorname{Im}(t_1-t_2)>-\beta$.

In the same time, using $1=\sum_m|m\rangle\langle m|$, we have

$$G^{>}(1,2)=$$
$$\exp[\beta\,\mu\,N]\left(\sum_n\exp[E_n(i\;t_1-i\,t_2-\beta)]\left\langle n\left|\psi(r_1)\sum_m\right|m\right\rangle\left\langle m\left|\exp\left(-i\,\hat{H}\,t_1\right)\exp\left(i\,\hat{H}\,t_2\right)\psi^{\dagger}(r_2)\right|n\right\rangle\right)\Big/\left(i\operatorname{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\right\}\right)=$$
$$\exp[\beta\,\mu\,N]\left(\sum_{n,m}\exp[E_n(i\;t_1-i\,t_2-\beta)]\left\langle n\,|\,\psi(r_1)\,|\,m\right\rangle\left\langle m\left|\psi^{\dagger}(r_2)\right|n\right\rangle\exp[i\,E_m(t_2-t_1)]\right)\Big/\left(i\operatorname{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\right\}\right) \tag{8.35}$$

To make sure that $E_m\to+\infty$ shows no singularity, $\operatorname{Im}(t_1-t_2)<0$.

So, $0>\operatorname{Im}(t_1-t_2)>-\beta$

For $G^{<}$, we have $0<\operatorname{Im}(t_1-t_2)<\beta$

Let's come back to $G^{>}$

$$G^{>}(r_1,\,t_1-i\,\beta;\,r_2,\,t_2)=$$
$$\frac{\operatorname{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\exp\left(\beta\,\hat{H}\right)\exp\left(i\,\hat{H}\,t_1\right)\psi(r_1)\exp\left(-i\,\hat{H}\,t_1\right)\exp\left(-\beta\,\hat{H}\right)\exp\left(i\,\hat{H}\,t_2\right)\psi^{\dagger}(r_2)\exp\left(-i\,\hat{H}\,t_2\right)\right\}}{i\operatorname{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\right\}}=$$
$$\frac{\operatorname{Tr}\left\{\exp\left[\beta\,\mu\,\hat{N}\right]\exp\left(i\,\hat{H}\,t_1\right)\psi(r_1)\exp\left(-i\,\hat{H}\,t_1\right)\exp\left(-\beta\,\hat{H}\right)\exp\left(i\,\hat{H}\,t_2\right)\psi^{\dagger}(r_2)\exp\left(-i\,\hat{H}\,t_2\right)\right\}}{i\operatorname{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\right\}}=$$
$$\frac{\operatorname{Tr}\left\{\exp\left(i\,\hat{H}\,t_1\right)\psi(r_1)\exp\left[\beta\,\mu\left(\hat{N}-1\right)\right]\exp\left(-i\,\hat{H}\,t_1\right)\exp\left(-\beta\,\hat{H}\right)\exp\left(i\,\hat{H}\,t_2\right)\psi^{\dagger}(r_2)\exp\left(-i\,\hat{H}\,t_2\right)\right\}}{i\operatorname{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\right\}}= \tag{8.36}$$

$$e^{-\beta\mu}\,\frac{\mathrm{Tr}\left\{\exp\left(i\,\hat{H}\,t_1\right)\psi(r_1)\exp\left(-i\,\hat{H}\,t_1\right)\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\exp\left(i\,\hat{H}\,t_2\right)\psi^\dagger(r_2)\exp\left(-i\,\hat{H}\,t_2\right)\right\}}{i\,\mathrm{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\right\}}=$$

$$e^{-\beta\mu}\,\frac{\mathrm{Tr}\left\{\psi(1)\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\psi^\dagger(2)\right\}}{i\,\mathrm{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\right\}}=e^{-\beta\mu}\,\frac{\mathrm{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\psi^\dagger(2)\,\psi(1)\right\}}{i\,\mathrm{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\,\hat{N}\right)\right]\right\}}=\pm e^{-\beta\mu}\,G^<(1,\,2)$$

So, $e^{\beta\,\mu}\,G^>(r_1,\,t_1-i\,\beta;\,r_2,\,t_2)=\pm\,G^<(r_1,\,t_1;\,r_2,\,t_2)$ (8.37)

8.2.2. BC for the time-ordered Green's function.

The time-ordered Green's function can be defined along the imaginary axis also

$$\begin{aligned}\mathcal{T}\,\psi(r_1,\,t_1)\,\psi^\dagger(r_2,\,t_2)&=\psi(r_1,\,t_1)\,\psi^\dagger(r_2,\,t_2)\quad\text{if }\mathrm{Im}(t_1)>\mathrm{Im}(t_2)\\&=\pm\psi^\dagger(r_2,\,t_2)\,\psi(r_1,\,t_1)\;\;\text{if }\mathrm{Im}(t_1)<\mathrm{Im}(t_2)\end{aligned}\tag{8.38}$$

So,

$$\begin{aligned}\mathcal{T}\,G&=G^>\quad\text{if }\mathrm{Im}(t_1)<\mathrm{Im}(t_2)\\&\pm G^<\;\;\text{if }\mathrm{Im}(t_1)>\mathrm{Im}(t_2)\end{aligned}\tag{8.39}$$

It is easy to check that for $G(r,\,t)$, we have

$$G(r,\,t)=\pm\,e^{\beta\mu}\,G(r,\,t-i\,\beta)\tag{8.40}$$

This is a boundary condition for imaginary time. At μ=0, Bosons have a periodic BC, and fermions have an anti-periodic BC.

8.2.3. the k,ω space

Define

$$\begin{aligned}G^>(k,\,\omega)&=i\int d\,r\,d\,t\,e^{-i\,k\,r+i\,\omega\,t}\,G^>(r,\,t)=\left\langle\psi_{k,\omega}\,\psi_{k,\omega}{}^\dagger\right\rangle\\G^<(k,\,\omega)&=\pm i\int d\,r\,d\,t\,e^{-i\,k\,r+i\,\omega\,t}\,G^<(r,\,t)=\left\langle\psi_{k,\omega}{}^\dagger\,\psi_{k,\omega}\right\rangle\end{aligned}\tag{8.41}$$

$$\begin{aligned}&G^<(k,\,\omega)=\pm i\int d\,r\,d\,t\,e^{-i\,k\,r+i\,\omega\,t}\,G^<(r,\,t)=\\&\quad i\,e^{\beta\,\mu}\int d\,r\,d\,t\,e^{-i\,k\,r+i\,\omega\,t}\,G^>(r,\,t-i\,\beta)=i\,e^{\beta\,\mu}\int d\,r\,d\,t'\,e^{-i\,k\,r+i\,\omega\,(t'+i\,\beta)}\,G^>(r,\,t')=e^{-\beta(\omega-\mu)}\,G^>(k,\,\omega)\end{aligned}\tag{8.42}$$

Define the "spectral function"

$$A(k,\,\omega)=G^>(k,\,\omega)\mp G^<(k,\,\omega)\tag{8.43}$$

Because $G^<(k,\,\omega)=e^{-\beta(\omega-\mu)}\,G^>(k,\,\omega)$

$$A(k,\,\omega)=G^>(k,\,\omega)\mp G^<(k,\,\omega)=G^>(k,\,\omega)\mp e^{-\beta(\omega-\mu)}\,G^>(k,\,\omega)\tag{8.44}$$

So

$$G^>(k,\,\omega)=\frac{A(k,\,\omega)}{1\mp e^{-\beta(\omega-\mu)}}=A(k,\,\omega)\,\frac{e^{\beta(\omega-\mu)}}{e^{\beta(\omega-\mu)}\mp1}=A(k,\,\omega)\left[1\pm\frac{1}{e^{\beta(\omega-\mu)}\mp1}\right]=A(k,\,\omega)[1\pm f(\omega)]\tag{8.45}$$

$$G^<(k,\,\omega)=e^{-\beta(\omega-\mu)}\,G^>(k,\,\omega)=e^{-\beta(\omega-\mu)}\,\frac{A(k,\,\omega)}{1\mp e^{-\beta(\omega-\mu)}}=A(k,\,\omega)\,\frac{1}{e^{\beta(\omega-\mu)}\mp1}=A(k,\,\omega)\,f(\omega)\tag{8.46}$$

Here $f(\omega)$ is the boson/fermion distribution function.

8.2.4. G in the k,ω space part I: the Matsubara frequencies

Remember that $G(r,\,t)=\pm\,e^{\beta\mu}\,G(r,\,t-i\,\beta)$, which is (almost) a PBC (anti-PBC) for t. We know that boundary conditions implies quantization (discrete ω).

For example, for a periodic function $f(t) = f(t+T)$, we know that in the frequency space, $f(\omega)$ is defined only on a discrete set of frequency points, $\omega = 2\pi n/T$. For anti-PBC, $f(t) = -f(t+T)$, $\omega = (2n+1)\pi/T$.

For $G(r, t) = \pm e^{\beta\mu} G(r, t - i\beta)$, if we go to the k,$\omega$ space and define

$$G(r, t) = \int d k\, d\omega\, e^{i k r - i\omega t} G(k, \omega) \tag{8.47}$$

The condition $G(r, t) = \pm e^{\beta\mu} G(r, t - i\beta)$ implies that

$$\int d k\, d\omega\, e^{i k r - i\omega t} G(k, \omega) = \pm e^{\beta\mu} e^{-\omega\beta} \int d k\, d\omega\, e^{i k r - i\omega t} G(k, \omega) \tag{8.48}$$

So, $\pm e^{\beta\mu} e^{-\omega\beta}=1$

$$e^{\beta(\omega-\mu)} = \pm 1 \tag{8.49}$$

For bosons,

$$\beta(\omega-\mu) = 2 n \pi i \tag{8.50}$$

$$\omega = \frac{2 n \pi i}{\beta} + \mu \tag{8.51}$$

Following the historical convention, we write $\omega = i\omega_n$

$$\omega_n = \frac{2 n \pi}{\beta} - i\mu \tag{8.52}$$

These discrete frequency points ω_n are known as the Matsubara frequencies

For fermions,

$$\beta(\omega-\mu) = (2n+1)\pi i \tag{8.53}$$

$$\omega = \frac{(2n+1)\pi i}{\beta} + \mu \tag{8.54}$$

$$\omega_n = \frac{2n+1}{\beta}\pi - i\mu \tag{8.55}$$

8.2.5. G in the k,ω space part II: analytic continuation

After we find $G(k, i\omega_n)$, where ω_n takes discrete values, now let's define a new function $G(k, z)$ by simply replacing the discrete number $i\omega_n$ into a complex number z that various continuously . For the function $G(k, z)$, it is a function well-defined at every point on the complex z plane (there may be some singularity points). At the Matsubara frequencies, this new function $G(k, z)$ coincides with $G(k, i\omega_n)$. This procedure is known as analytic continuation. This new function is very useful. Here, I will show you that by defining $G(k, z)$, we can find a very easy way to get $G^>$ and $G^<$ from G. Later, we will use this $G(k, z)$ to compute $G(k, i\omega_n)$.

$$G(k, i\omega_n) = \int_0^{-i\beta} d t\, e^{-\omega_n t} G(k, t) =$$
$$\int_0^{-i\beta} d t\, e^{-\omega_n t} G^>(k, t) = \int_0^{-i\beta} d t\, e^{-\omega_n t} \int \frac{d\omega}{2\pi i} e^{-i\omega t} G^>(k, \omega) = \int \frac{d\omega}{2\pi} \frac{e^{(-i\omega-\omega_n)(-i\beta)} - 1}{\omega - i\omega_n} \frac{A(k, \omega)}{1 \mp e^{-\beta(\omega-\mu)}} =$$
$$\int \frac{d\omega}{2\pi} \frac{1 - e^{-(\omega - i\omega_n)\beta}}{\omega - i\omega_n} \frac{A(k, \omega)}{1 \mp e^{-\beta(\omega-\mu)}} = \int \frac{d\omega}{2\pi} \frac{1 \mp e^{-(\omega-\mu)\beta}}{i\omega_n - \omega} \frac{A(k, \omega)}{1 \mp e^{-\beta(\omega-\mu)}} = \int \frac{d\omega}{2\pi} \frac{A(k, \omega)}{i\omega_n - \omega} \tag{8.56}$$

Therefore,

$$G(k, z) = \int \frac{d\omega}{2\pi} \frac{A(k, \omega)}{z - \omega} \tag{8.57}$$

Now, we substitute z by $\omega + i\delta$

$$G(k,\ \omega + i\,\epsilon) = \int \frac{d\,\Omega}{2\,\pi}\ \frac{A(k,\ \Omega)}{\omega + i\,\epsilon - \Omega} \tag{8.58}$$

$$\begin{aligned}\operatorname{Im}[G(k,\ \omega + i\,\epsilon)] &= \frac{G(k,\ \omega + i\,\epsilon) - G(k,\ \omega - i\,\epsilon)}{2\,i} = \frac{1}{2\,i}\int \frac{d\,\Omega}{2\,\pi}\left[\frac{A(k,\ \Omega)}{\omega + i\,\epsilon - \Omega} - \frac{A(k,\ \Omega)}{\omega - i\,\epsilon - \Omega}\right] = \\ &\frac{1}{2\,i}\int \frac{d\,\Omega}{2\,\pi}\ \frac{A(k,\ \Omega)}{(\omega - \Omega)^2 + \epsilon^2}(-2\,i\,\epsilon) = -\int \frac{d\,\Omega}{2\,\pi}\ \frac{\epsilon}{(\omega - \Omega)^2 + \epsilon^2}\,A(k,\ \Omega) = -\frac{1}{2}\int d\,\Omega\,\delta(\omega - \Omega)\,A(k,\ \Omega) = -\frac{1}{2}\,A(k,\ \omega)\end{aligned} \tag{8.59}$$

So,

$$A(k,\ \omega) = -2\,\operatorname{Im}[G(k,\ \omega + i\,\epsilon)] \tag{8.60}$$

8.2.6. Example: free particles

$$i\,\partial_t\,G_0(r.t) + \frac{1}{2\,m}\,\nabla^2\,G_0(r,\ t) = \ \delta(r)\,\delta(t) \tag{8.61}$$

in the k,ω space

$$\left(i\,\omega_n - \frac{k^2}{2\,m}\right)G_0(k,\ i\,\omega_n) = \ 1 \tag{8.62}$$

$$G_0(k,\ i\,\omega_n) = \ \frac{1}{i\,\omega_n - \frac{k^2}{2\,m}} \tag{8.63}$$

More generic case: dispersion relation ϵ(k)

$$G_0(k,\ i\,\omega_n) = \ \frac{1}{i\,\omega_n - \epsilon(k)} \tag{8.64}$$

Analytic continuation:

$$G_0(k,\ z) = \ \frac{1}{z - \epsilon(k)} \tag{8.65}$$

the spectral function:

$$A(k,\ \omega) = -2\,\operatorname{Im}[G(k,\ \omega + i\,\epsilon)] = -2\,\operatorname{Im}\left[\frac{1}{\omega + i\,\epsilon - \epsilon(k)}\right] = \frac{2\,\epsilon}{(\omega - \epsilon_k)^2 + \epsilon^2} = 2\,\pi\,\delta(\omega - \epsilon_k) \tag{8.66}$$

particular number:

$$\langle n_k(t)\rangle = \left\langle {\psi_k}^\dagger(t)\,\psi_k(t)\right\rangle = G^<(k,\ t - t) = \int \frac{d\,\omega}{2\,\pi}\ G^<(k,\ \omega) = \int \frac{d\,\omega}{2\,\pi}\ 2\,\pi\,\delta(\omega - \epsilon_k)\ f(\omega) = f(\epsilon_k) \tag{8.67}$$

$$\langle 1 \pm n_k(t)\rangle = \left\langle \psi_k(t)\,{\psi_k}^\dagger(t)\right\rangle = G^>(k,\ t - t) = \int \frac{d\,\omega}{2\,\pi}\ G^>(k,\ \omega) = \int \frac{d\,\omega}{2\,\pi}\ 2\,\pi\,\delta(\omega - \epsilon_k)[1 \pm f(\omega)] = 1 \pm f(\epsilon_k) \tag{8.68}$$

8.2.7. Interacting particles.

Once we found $G(k,\ i\omega_n)$,

We can get $A(k,\ \omega)$ using

$$A(k,\ \omega) = -2\,\operatorname{Im}[G(k,\ \omega + i\,\epsilon)] \tag{8.69}$$

Then we can get all other correlation functions like $G^<(k,\ t - t)$ and $G^>(k,\ t - t)$ using

$$G^>(k,\ \omega) = \frac{A(k,\ \omega)}{1 \mp e^{-\beta(\omega - \mu)}} = A(k,\ \omega)\ \frac{e^{\beta(\omega - \mu)}}{e^{\beta(\omega - \mu)} \mp 1} = A(k,\ \omega)\left[1 \pm \frac{1}{e^{\beta(\omega - \mu)} \mp 1}\right] = A(k,\ \omega)[1 \pm f(\omega)] \tag{8.70}$$

$$G^{<}(k,\ \omega) = e^{-\beta(\omega-\mu)}\, G^{>}(k,\ \omega) = e^{-\beta(\omega-\mu)}\, \frac{A(k,\ \omega)}{1 \mp e^{-\beta(\omega-\mu)}} = A(k,\ \omega)\, \frac{1}{e^{\beta(\omega-\mu)} \mp 1} = A(k,\ \omega)\, f(\omega) \tag{8.71}$$

8.2.8. Other particles (free particles only in this section)

For free particles, the Green's function has the same equation of motion as the wavefunction, but with an extra δ-function.

For particles that follow the Schrödinger equation,

$$i\,\partial_t \psi = -\frac{\nabla^2}{2\,m}\psi \tag{8.72}$$

$$\left(i\,\partial_t + \frac{\nabla^2}{2\,m}\right)\psi = 0 \tag{8.73}$$

The Green's function has the same EMO, but with a δ-function on the r.h.s.

$$\left(i\,\partial_t + \frac{\nabla^2}{2\,m}\right) G(r,\ t) = \delta(r)\,\delta(t) \tag{8.74}$$

If we go to k-space,

$$(\omega - \epsilon_k)\, G(k,\ \omega) = 1 \tag{8.75}$$

$$G(k,\ \omega) = \frac{1}{\omega - \epsilon_k} \tag{8.76}$$

In some sense, the Green's function is just the inverse of the EOM

$$G(r,\ t) = \left(i\,\partial_t + \frac{\nabla^2}{2\,m}\right)^{-1} \tag{8.77}$$