Lecture 9

 Imaginary time formalism

Recall our definition of the time ordered Green's function in the momentum space representation $\hat{H} = \hat{H} - \mu\hat{N}$ here

$$g_\sigma(\bar{k}, t, t') = -i\,\mathrm{Tr}\{e^{-\beta H}\, T\, c_{k\sigma}(t)\, c^\dagger_{k\sigma}(t')\}\,\frac{1}{Z}$$

$$= -i\,\mathrm{Tr}\{e^{-\beta H}\, T\, e^{iHt} c_{k\sigma} e^{-iHt}\; e^{iHt'} c^\dagger_{k\sigma} e^{-iHt'}\}\,\frac{1}{Z}$$

Note how we have exponentials with statistical factors $e^{-\beta H}$ and with time evolution factors $e^{\pm iHt}$. If we instead examined functions of imaginary time $\tau = it$, we could have all exponential phases go to exponential decay and everything would be well defined. This procedure is called a <u>wick rotation</u>.

This is the basic idea behind the imaginary time formalism.

Define Green's functions via the following with $|\tau| \leq \beta$

$$G_\sigma(\bar{k}, \tau, \tau') = -\mathrm{Tr}\,\{e^{-\beta H}\, T_\tau\, c_{k\sigma}(\tau)\, c^\dagger_{k\sigma}(\tau')\}\,\frac{1}{Z}$$

(where the generalization to real space is obvious)

Here $\quad c_{k\sigma}(\tau) = e^{\tau H} c_{k\sigma} e^{-\tau H} \qquad c^\dagger_{k\sigma}(\tau) = e^{\tau H} c^\dagger_{k} e^{-\tau H}$

Note, not the Hermitian conjugate any more!

The T_τ denotes time ordering with respect to imaginary time.

$\boxed{\text{Property 1} \quad G_\sigma(\vec{k}, \tau, \tau') = G_\sigma(\vec{k}, \tau - \tau')}$

Proof: consider $\tau > \tau'$ then

$$G_\sigma(\vec{k}, \tau, \tau') = -\mathrm{Tr}\, \{e^{-\beta H} e^{\tau H} c_{k\sigma} e^{-\tau H} e^{\tau' H} c^+_{k\sigma} e^{-\tau' H}\}/Z$$

$$= -\mathrm{Tr}\, \{e^{-\tau' H} e^{-\beta H} e^{\tau H} c_{k\sigma} e^{-(\tau-\tau')H} c^+_{k\sigma}\}/Z$$

since $\mathrm{Tr}[AB] = \sum_{mn} A_{mn} B_{nm} = \mathrm{Tr}(BA)$

$$= -\mathrm{Tr}\, \{e^{-\beta H} e^{(\tau-\tau')H} c_{k\sigma} e^{-(\tau-\tau')H} c^+_{k\sigma}\}/Z$$

since $e^{-\beta H}$ and $e^{-\tau' H}$ commute

$$= G_\sigma(\vec{k}, \tau - \tau', 0) \qquad \text{since } \tau > \tau'$$

one can do a similar proof for $\tau < \tau'$.

$\Rightarrow$ G is a function only of $\tau - \tau'$.

We assume the spectrum of H is positive, then all exponential factors are well defined as long as $|\tau - \tau'| \leq \beta$ since the $e^{-\beta H}$ factor always wins over $e^{\pm(\tau-\tau')H}$.

$\boxed{\text{Property 2: } G_\sigma(\vec{k}, \tau) = -G_\sigma(k, \tau - \beta) \quad \text{for } 0 \leq \tau \leq \beta}$

Proof: $G_\sigma(\vec{k}, \tau) = -\mathrm{Tr}\, \{e^{-\beta H} e^{\tau H} c_{k\sigma} e^{-\tau H} c^+_{k\sigma}\}/Z$ for $0 \leq \tau \leq \beta$

$$= -\mathrm{Tr}\, \{e^{-\tau H} c^+_{k\sigma} e^{-\beta H} e^{\tau H} c_{k\sigma}\}/Z$$ by cyclic property of trace

$$= -\mathrm{Tr}\, \{\underbrace{e^{-\beta H} e^{\beta H}}_{1} e^{-\tau H} c^+_{k\sigma} e^{-\beta H} e^{\tau H} c_{k\sigma}\}/Z$$

$$= -\mathrm{Tr}\, \{\underbrace{e^{-\beta H} e^{(\beta-\tau)H}}_{\text{commute}} c^+_{k\sigma} e^{-(\beta-\tau)H} c_{k\sigma}\}/Z$$

$$= -\mathrm{Tr}\left\{ e^{\cancel{\beta H}(\beta-\tau)H} e^{-\beta H} c^{\dagger}_{\vec{k}\sigma} e^{-(\beta-\tau)H} c_{\vec{k}\sigma} \right\}/Z$$

$$= -\mathrm{Tr}\left\{ e^{-\beta H} c^{\dagger}_{\vec{k}\sigma} e^{-(\beta-\tau)H} c_{\vec{k}\sigma} e^{(\beta-\tau)H} \right\}/Z$$

note if $0 \le \cancel{\beta}\tau \le \beta$ $\quad -(\beta-\tau) < 0$

$$= -\mathrm{Tr}\left\{ e^{-\beta H} T_\tau\, c^{\dagger}_{\vec{k}\sigma}(0) c_{\vec{k}\sigma}(-\beta+\tau) \right\}/Z$$

$$= -G_\sigma(\vec{k}, -(\beta-\tau))$$

minus sign from time ordering in original definition of G_σ

so $\quad G_\sigma(\vec{k},\tau) = -G_\sigma(\vec{k},\tau-\beta)$

$\Rightarrow$ G is <u>antiperiodic</u> with period β. Also called the boundary condition.

This allows us to extend the definition of G to all τ by using the antiperiodicity property.

So for $|\tau| > \beta$ we let $G_\sigma(\vec{k},\tau) = -G_\sigma(\vec{k},\tau-\beta)$ and repeat until final τ is less than β in magnitude.

Since it is antiperiodic, we expand in a Fourier series

$$G_\sigma(\vec{k},\tau) = T \sum_n e^{-i\omega_n\tau} G_\sigma(\vec{k}, i\omega_n)$$

$\uparrow$ temperature not time ordering.

with $G_\sigma(\vec{k}, i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau} G_\sigma(\vec{k},\tau)$

and $i\omega_n = i\pi T(2n+1)$ $\quad n =$ integer $\quad$ called a <u>Matsubara</u> <u>frequency</u>.

check the antiperiodicity!

$$G_0(\vec{k},\tau-\beta) = T\sum_n e^{-i\omega_n(\tau-\beta)}\,G_0(\vec{k},i\omega_n)$$

$$= -T\sum_n e^{-i\omega_n\tau}\,G_0(\vec{k},i\omega_n) \quad \text{since } e^{-i\omega_n\beta} = -1$$

$$= -G_0(\vec{k},\tau) \quad \checkmark$$

Definition of the self-energy

We use Dyson's equation to define the self-energy

$$\boxed{G_0(\vec{k},i\omega_n) = \frac{1}{i\omega_n + \mu - \underbrace{\Sigma(k,i\omega_n)}_{\text{self-energy fcn of } \vec{k} \text{ and } i\omega_n} - \varepsilon_k}} \qquad \varepsilon_k = \text{band structure}$$

The self-energy determines how G deviates from the noninteracting GF.
The sign of the imaginary part of G is the same as the sign of the imaginary part of Σ.

It is often much easier to calculate Green's functions on the imaginary axis than on the real axis. All static properties (zero frequency or time independent) can be found from the imaginary axis formalism. Dynamical properties require more work.

Analytic continuation

Both the GF and the self-energy are known on an infinite set of points ($i\omega_n$) in the complex plane. They also are bounded (decay like $\frac{1}{i\omega_n}$ as $|i\omega_n| \to \infty$ for the self-energy this is true when a constant is subtracted).

It turns out there is a unique analytic continuation of this function in the complex UHP or LHP. This analytic continuation can be used to define it on the real axis. The boundedness at infinity is crucial for this to work.

We want to show how to go from the time-ordered GF on the imaginary axis to the retarded GF on the real axis by working in the UHP.

To do this, we need to recall our Lehmann representation for $g^R(k,\omega)$

$$g^R(k,\omega) = -i \int_{-\infty}^{+\infty} dt \; \theta(t) \langle [c_k(t), c_k^\dagger(0)]_+ \rangle e^{i\omega t}$$

$$= -i \int_0^\infty dt \, e^{i\omega t} \sum_{mn} \Big\{ \langle m|c_k|n\rangle \langle n|c_k^\dagger|m\rangle \rho_m e^{i(E_m-E_n)t} + \langle m|c_k^\dagger|n\rangle \langle n|c_k|m\rangle \rho_m e^{i(E_n-E_m)t} \Big\}$$

$$= -i \int_0^\infty dt \, e^{i\omega t} \sum_{mn} |\langle m|c_k|n\rangle|^2 (\rho_m+\rho_n) e^{i(E_m-E_n)t}$$

regularize by $\omega \to \omega + i\delta \quad \delta \to 0^+$

$$= \sum_{mn} \frac{1}{\omega + E_m - E_n + i\delta} (\rho_m+\rho_n) |\langle m|c_k|n\rangle|^2$$

This function is analytic for all ω in the UHP. evaluate at the Matsubara frequencies

$$g^R(\vec{k}, i\omega_{n'}) = \sum_{mn} \frac{1}{i\omega_{n'} + E_m - E_n} (\rho_m + \rho_n) |\langle m | c_k | n \rangle|^2$$

But

$$G(k, i\omega_{n'}) = \int_0^\beta d\tau \, e^{i\omega_{n'}\tau} G(\vec{k}, \tau)$$

$$= -\int_0^\beta d\tau \, e^{i\omega_{n'}\tau} \sum_{mn} \langle m | e^{-\beta H} e^{\tau H} c_k e^{-\tau H} | n \rangle \langle n | c_k^\dagger | m \rangle / Z$$

corrected 9-18-2012

$$= -\int_0^\beta d\tau \, e^{i\omega_{n'}\tau} \sum_{mn} \rho_m e^{\tau(E_m - E_n)} |\langle m | c_k | n \rangle|^2$$

$$= -\sum_{mn} \rho_m |\langle m | c_k | n \rangle|^2 \int_0^\beta d\tau \, e^{(i\omega_{n'} + E_m - E_n)\tau}$$

$$= -\sum_{mn} \rho_m |\langle m | c_k | n \rangle|^2 \left. \frac{e^{(i\omega_{n'} + E_m - E_n)\tau}}{i\omega_{n'} + E_m - E_n} \right|_0^\beta$$

$$= \sum_{mn} \rho_m \left(e^{\beta(E_m - E_n)} + 1 \right) \frac{|\langle m | c_k | n \rangle|^2}{i\omega_{n'} + E_m - E_n} \quad \text{since } e^{i\omega_n \beta} = -1$$

But $\rho_m e^{\beta(E_m - E_n)} = \rho_n$ so

$$= \sum_{mn} \frac{1}{i\omega_{n'} + E_m - E_n} (\rho_m + \rho_n) |\langle m | c_k | n \rangle|^2$$

which is identical to $g^R(\vec{k}, i\omega_n)$!

This implies

$$g^R(\vec{k}, z)$$

is analytic in the UHP, is bounded as $|z| \to \infty$ and it agrees with $G(\vec{k}, i\omega_n)$ for all $n \geq 0$

This must be the <u>unique</u> analytic continuation from the theorem.

Hence $$G(\vec{k}, i\omega_n) = \int d\omega \frac{A(\vec{k}, \omega)}{i\omega_n - \omega}$$

since this is the formula we found for G^+ in the UHP.

Note, since $\int d\omega A(\vec{k}, \omega) = 1$, we immediately see

$G(\vec{k}, i\omega_n)$ decays like $\frac{1}{i\omega_n}$ for large ω_n.