Imaginary time
Green’s function

Alex Taekyung Lee
Nonzero temperature

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• The exact state of all these other particles is not known, since they are fluctuating between different configurations.
Nonzero temperature

- At nonzero temperature => Particle may interact with a bath of other particles which have an average energy.
- The exact state of all these other particles is not known, since they are fluctuating between different configurations.
- All we know: temperature = mean energy.
- => Green’s function should be averaged.

\[
C_{AB}(t, t') = -\langle A(t)B(t') \rangle = -\frac{1}{Z} \text{Tr}(e^{-\beta H} A(t)B(t'))
\]

where \( Z = Tr[e^{-\beta H}] \)
Imaginary time and Matsubara green’s function

From the real-time Heisenberg picture:

\[ A(t) = e^{itH} A e^{-itH} \]

Replace it => \( \tau \):

\[ A(\tau) = e^{\tau H} A e^{-\tau H}, \quad \text{Heisenberg} \]
\[ A_I(\tau) = e^{\tau H_0} A e^{-\tau H_0}, \quad \text{Interaction} \]

\[ U_I(\tau, \tau') = e^{\tau H_0} e^{-(\tau-\tau')H} e^{-\tau' H_0} = T_\tau \exp\left(-\int_{\tau'}^{\tau} d\tau_1 V_I(\tau_1)\right) \]

\[ e^{-\beta H} = e^{-\beta H_0} U_I(\beta, 0) = e^{-\beta H_0} T_\tau \exp\left(-\int_{0}^{\beta} d\tau_1 V_I(\tau_1)\right) \]
Imaginary time and Matsubara green’s function

- From the real-time heisenberg picture: \[ A(t) = e^{itH} Ae^{-itH} \]

- Replace it \( \Rightarrow \tau \):
  \[ A(\tau) = e^{\tau H} Ae^{-\tau H}, \quad \text{Heisenberg} \]
  \[ A_I(\tau) = e^{\tau H_0} Ae^{-\tau H_0}, \quad \text{Interaction} \]

- **Matsubara Green’s function**: for \( 0 < \tau, \tau' < \beta \)
  \[ C_{AB}(\tau, \tau') \equiv -\langle T_{\tau}[A(\tau)B(\tau')] \rangle \]

- Time ordering operator:
  \[ T_{\tau} (A(\tau)B(\tau')) = \theta(\tau - \tau') A(\tau)B(\tau') \pm \theta (\tau' - \tau) B(\tau')A(\tau), \quad \{ + \text{ for bosons, } - \text{ for fermions.} \} \]
Properties of Matsubara green’s function

1. $C_{AB}$ only depends on $\tau - \tau'$:

$$C_{AB}(\tau, \tau') = C_{AB}(\tau - \tau').$$

$$C_{AB}(\tau, \tau') = \frac{-1}{Z} \text{Tr}[e^{-\beta H}e^{\tau H}Ae^{-\tau H}e^{\tau'H}Be^{-\tau'H}]$$

$$= \frac{-1}{Z} \text{Tr}[e^{-\beta H}e^{(\tau-\tau')H}Ae^{-(\tau-\tau')H}B] = C_{AB}(\tau - \tau') \quad \text{for} \quad \tau > \tau'.$$
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$$= \frac{-1}{Z} \text{Tr}[e^{-\beta H} e^{(\tau-\tau')H} A e^{-(\tau-\tau')H} B] = C_{AB}(\tau - \tau') \text{ for } \tau > \tau'.$$

2. $C_{AB}(\tau - \tau')$ is naturally defined in the interval of $-\beta < \tau - \tau' < \beta$. Otherwise it diverges. It is clear if we consider Lehman representation for $\tau > \tau'$

$$C_{AB}(\tau - \tau') = \frac{-1}{Z} \sum_{n,n'}[e^{-\beta E_n} e^{(\tau-\tau')E_n} A_{nn'} e^{-(\tau-\tau')E_n'} B_{n'n}]$$
Properties of Matsubara green’s function

3. $C_{AB}(\tau)$ is periodic with period $\beta$, $C_{AB}(\tau) = \pm C_{AB}(\tau + \beta)$

Consider the case of $-\beta < \tau < 0$:

$$C_{AB}(\tau) = \pm \frac{-1}{Z} \text{Tr}[e^{-\beta H}Be^{\tau H}Ae^{-\tau H}] = \pm \frac{-1}{Z} \text{Tr}[e^{\tau H}Ae^{-(\beta+\tau)H}B]$$

$$= \pm \frac{-1}{Z} \text{Tr}[e^{-\beta H}e^{(\tau+\beta)H}Ae^{-(\beta+\tau)H}B] = \pm C_{AB}(\tau + \beta).$$
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Using imaginary time

$\Rightarrow$ we can treat temperature as time!
Fourier transform of Matsubara green’s function

• As $C_{AB}$ is defined for $-\beta < \tau < \beta$, desecrate Fourier transform is defined as

$$C_{AB}(n) \equiv \frac{1}{2} \int_{-\beta}^{\beta} d\tau e^{in\tau/\beta} C_{AB}(\tau),$$

$$C_{AB}(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-in\tau/\beta} C_{AB}(n).$$

• They become

$$C_{AB}(n) = \int_{0}^{\beta} d\tau e^{in\tau/\beta} C_{AB}(\tau), \quad \left\{ \begin{array}{l} n \text{ is even for bosons,} \\
 n \text{ is odd for fermions.} \end{array} \right.$$  

$$C_{AB}(i\omega_n) = \int_{0}^{\beta} d\tau e^{i\omega_n\tau} C_{AB}(\tau), \quad \left\{ \begin{array}{l} \omega_n = \frac{2n\pi}{\beta}, \quad \text{for bosons,} \\
 \omega_n = \frac{(2n+1)\pi}{\beta}, \quad \text{for fermions.} \end{array} \right.$$  

• $\omega_n$ is called as Matsubara frequency
Example: non interacting particle

• Single particle Matsubara Green’s function:

\[
G(r\sigma\tau, r'\sigma'\tau') = -\left\langle T_{\tau} \left( \Psi_\sigma(r, \tau) \Psi_\sigma^\dagger(r', \tau') \right) \right\rangle, \quad \text{real space,}
\]
\[
G(\nu\tau, \nu'\tau') = -\left\langle T_{\tau} \left( c_\nu(\tau) c_\nu^\dagger(\tau') \right) \right\rangle, \quad \{\nu\} \text{ representation.}
\]

• Consider a Hamiltonian: \( H_0 = \sum_\nu \xi_\nu c_\nu^\dagger c_\nu \).
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- Consider a Hamiltonian:

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H_0 = \sum_\nu \xi_\nu c_\nu^\dagger c_\nu,
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c_\nu(\tau) = e^{\tau H_0} c_\nu e^{-\tau H_0} = e^{-\xi_\nu \tau} c_\nu, \quad c_\nu^\dagger(\tau) = e^{\tau H_0} c_\nu^\dagger e^{-\tau H_0} = e^{\xi_\nu \tau} c_\nu^\dagger,
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- Consider a Hamiltonian:

$$H_0 = \sum_\nu \xi_\nu c_\nu^\dagger c_\nu,$$

$$c_\nu(\tau) = e^{\tau H_0} c_\nu e^{-\tau H_0} = e^{-\xi_\nu \tau} c_\nu, \quad c_\nu^\dagger(\tau) = e^{\tau H_0} c_\nu^\dagger e^{-\tau H_0} = e^{\xi_\nu \tau} c_\nu^\dagger,$$

$$G_0(\nu, \tau - \tau') = - \left\langle T_\tau \left( c_\nu(\tau) c_\nu^\dagger(\tau') \right) \right\rangle,$$

$$= - \theta(\tau - \tau') \langle c_\nu(\tau) c_\nu^\dagger(\tau') \rangle - (\pm) \theta(\tau' - \tau) \langle c_\nu^\dagger(\tau') c_\nu(\tau) \rangle$$

$$= - \left[ \theta(\tau - \tau') \langle c_\nu c_\nu^\dagger \rangle (\pm) \theta(\tau' - \tau) \langle c_\nu^\dagger c_\nu \rangle \right] e^{-\xi_\nu (\tau - \tau')}.$$
Example: non interacting particle

• For fermion:

\[ G_{0,F}(\nu, \tau - \tau') = - \left[ \theta(\tau - \tau')(1 - n_F(\xi_\nu)) - \theta(\tau' - \tau)n_F(\xi_\nu) \right] e^{-\xi_\nu(\tau - \tau')} \]

\[ G_{0,F}(\nu, ik_n) = \int_{0}^{\beta} d\tau e^{ik_n\tau} G_{0,F}(\nu, \tau), \quad k_n = (2n + 1) \pi/\beta \]

\[ = \frac{1}{ik_n - \xi_\nu} \]

\[ n_F = \langle c_\nu^\dagger c_\nu \rangle = \frac{1}{e^{\beta \xi} + 1} \]
Example: non interacting particle

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= \frac{1}{ik_n - \xi_\nu}
\]

\[
n_F = < c^\dagger_\nu c_\nu > = \frac{1}{e^{\beta \xi} + 1}
\]

• For boson:

\[
G_{0,B}(\nu, \tau - \tau') = - [\theta(\tau - \tau') (1 + n_B(\xi_\nu)) + \theta(\tau' - \tau) n_B(\xi_\nu)] e^{-\xi_\nu(\tau - \tau')}
\]

\[
G_{0,B}(\nu, iq_n) = \int_0^\beta d\tau e^{iq_n \tau} G_{0,B}(\nu, \tau), \quad q_n = 2n\pi / \beta
\]

\[
= \frac{1}{iq_n - \xi_\nu}
\]
Example: non interacting particle

- Combine $q_n$ and $k_n$ to $\omega_n$:

- $\omega_n = n\pi/\beta$ (n=odd: fermion, n=even: boson)

\[ G_0(\nu, i\omega_n) = \frac{1}{i\omega_n - \xi_\nu} \]

- Using analytic continuation:

\[ G_0(\nu, i\omega_n \rightarrow \omega + i\eta) = \frac{1}{\omega - \xi_\nu + i\eta} = G_0^R(\omega) \]
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Figure from Bruus and Flensberg
Reference

• Many-Particle Physics, Mahan
• Many-Body Quantum Theory in Condensed Matter Physics, Bruus and Flensberg
Appendix
The Schrödinger picture

\[
\begin{align*}
\text{states:} & \quad |\psi(t)\rangle = e^{-iHt} |\psi_0\rangle, \\
\text{operators:} & \quad A, \text{ may or may not depend on time.} \\
& \quad H, \text{ does not depend on time.}
\end{align*}
\]
Interaction picture

The Schrödinger picture

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$$ operators: \quad A, \text{ may or may not depend on time.}$$

$$ H, \text{ does not depend on time.}$$

The Heisenberg picture

$$ state: \quad |\psi_0\rangle \equiv e^{iHt} |\psi(t)\rangle,$$

$$ operators: \quad A(t) \equiv e^{iHt} A e^{-iHt}.$$
**Interaction picture**

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& \quad H, \text{ does not depend on time.}
\end{align*}
\]

- **Interaction picture:** separate time evolution due to $H_0$ and $V$ \[ H = H_0 + V \]

The interaction picture

\[
\begin{align*}
\text{states:} & \quad |\hat{\psi}(t)\rangle \equiv e^{iH_0 t} |\psi(t)\rangle, \\
\text{operators:} & \quad \hat{A}(t) \equiv e^{iH_0 t} A e^{-iH_0 t}. \\
& \quad H_0, \text{ does not depend on time.}
\end{align*}
\]

\[ |\hat{\psi}(t)\rangle = \hat{U}(t, t_0) |\hat{\psi}(t_0)\rangle \quad \text{U: unitary} \]
Imaginary time (1)

- From the real-time heisenberg picture:
  \[ A(t) = e^{itH} A e^{-itH} \]

- Replace it => \( \tau \):
  \[ A(\tau) = e^{\tau H} A e^{-\tau H}, \quad \text{Heisenberg} \]
  \[ A_I(\tau) = e^{\tau H_0} A e^{-\tau H_0}, \quad \text{Interaction} \]
  \[ U_I(\tau, \tau') = e^{\tau H_0} e^{-(\tau - \tau')H} e^{-\tau' H_0} = T_\tau \exp\left( - \int_{\tau'}^{\tau} d\tau_1 V_I(\tau_1) \right) \]

- The thermal average is written, in terms of \( U_I(\tau, \tau') \):
  \[ e^{-\beta H} = e^{-\beta H_0} U_I(\beta, 0) = e^{-\beta H_0} T_\tau \exp\left( - \int_{0}^{\beta} d\tau_1 V_I(\tau_1) \right) \]
For example, consider the averaged correlation function with imaginary time:

\[ \langle T_\tau A(\tau)B(\tau') \rangle = \frac{1}{Z} \text{Tr}\{e^{-\beta H} T_\tau [A(\tau)B(\tau')]\} \]

\[ = \frac{1}{Z} \text{Tr}\{e^{-\beta H_0} T_\tau (U_I(\beta,0)A_I(\tau)B_I(\tau'))\} \]

\[ = \frac{\langle T_\tau (U_I(\beta,0)A_I(\tau)B_I(\tau'))\rangle_0}{\langle U_I(\beta,0)\rangle_0} \]

where we have:

\[ Z = \text{Tr}[e^{-\beta H_0} U_I(\beta,0)] = Z_0 \langle U_I(\beta,0)\rangle_0 \]

\[ Z_0 = \text{Tr} e^{-\beta H_0} \]
Fourier transform of Matsubara green’s function

\[ C_{AB}(n) = \frac{1}{2} \int_{0}^{\beta} d\tau \, e^{i\pi n\tau/\beta} C_{AB}(\tau) + \frac{1}{2} \int_{-\beta}^{0} d\tau \, e^{i\pi n\tau/\beta} C_{AB}(\tau), \]

\[ = \frac{1}{2} \int_{0}^{\beta} d\tau \, e^{i\pi n\tau/\beta} C_{AB}(\tau) + e^{-i\pi n} \frac{1}{2} \int_{0}^{\beta} d\tau \, e^{i\pi n\tau/\beta} C_{AB}(\tau - \beta), \]

\[ = \frac{1}{2} \left( 1 \pm e^{-i\pi n} \right) \int_{0}^{\beta} d\tau \, e^{i\pi n\tau/\beta} C_{AB}(\tau), \]

The factor \( 1 \pm e^{-i\pi n} \) is zero for + (bosons) and odd \( n \), or for - (fermions) and even \( n \).
Example: non interacting particle

• For fermion:

\[ G_{0,F}(\nu, i k_n) = \int_0^\beta d\tau \ e^{i k_n \tau} G_{0,F}(\nu, \tau), \quad k_n = (2n + 1) \pi / \beta \]

\[ = - (1 - n_F(\xi_\nu)) \int_0^\beta d\tau \ e^{i k_n \tau} e^{-\xi_\nu \tau}, \]

\[ = - (1 - n_F(\xi_\nu)) \frac{1}{i k_n - \xi_\nu} \left( e^{i k_n \beta} e^{-\xi_\nu \beta} - 1 \right), \]

\[ = \frac{1}{i k_n - \xi_\nu}, \]

because \( e^{i k_n \beta} = -1 \) and \( 1 - n_F(\varepsilon) = \left( e^{-\beta \varepsilon} + 1 \right)^{-1}. \)
Example: non interacting particle

- For boson:

\[ g_{0,B}(\nu, iq_n) = \int_0^\beta d\tau e^{iq_n \tau} g_{0,B}(\nu, \tau), \quad q_n = 2n\pi/\beta \]

\[ = - (1 + n_B(\xi_\nu)) \int_0^\beta d\tau e^{iq_n \tau} e^{-\xi_\nu \tau}, \]

\[ = - (1 + n_B(\xi_\nu)) \frac{1}{iq_n - \xi_\nu} \left( e^{iq_n \beta} e^{-\xi_\nu \beta} - 1 \right) \]

\[ = \frac{1}{iq_n - \xi_\nu}, \]

using \( e^{iq_n \beta} = 1 \) and \( 1 + n_B(\varepsilon) = - \left( e^{-\beta \varepsilon} - 1 \right)^{-1}. \)
Various Green’s functions

1. Retarded Green function

\[ G^R(r\sigma t, r'\sigma' t') = -i\theta(t-t')\langle [\hat{\Psi}_\sigma(rt), \hat{\Psi}^\dagger_{\sigma'}(r't')] \rangle_{\pm} \]

2. Advanced Green function

\[ G^A(r\sigma t, r'\sigma' t') = i\theta(t' - t)\langle [\hat{\Psi}_\sigma(rt), \hat{\Psi}^\dagger_{\sigma'}(r't')] \rangle_{\pm}. \]

3. Greater Green function

\[ G^{>}(r\sigma t, r'\sigma' t) = -i\langle \hat{\Psi}_\sigma(rt)\hat{\Psi}^\dagger_{\sigma'}(r't') \rangle, \]

4. Lesser Green function

\[ G^{<}(r\sigma t, r'\sigma' t) = +i\langle \hat{\Psi}^\dagger_{\sigma'}(r't')\hat{\Psi}_{\sigma}(rt) \rangle, \]

5. Time-ordered Green function

\[ G^t(r\sigma t, r'\sigma' t') = -i\langle T\hat{\Psi}_\sigma(rt)\hat{\Psi}^\dagger_{\sigma'}(r't') \rangle, \]