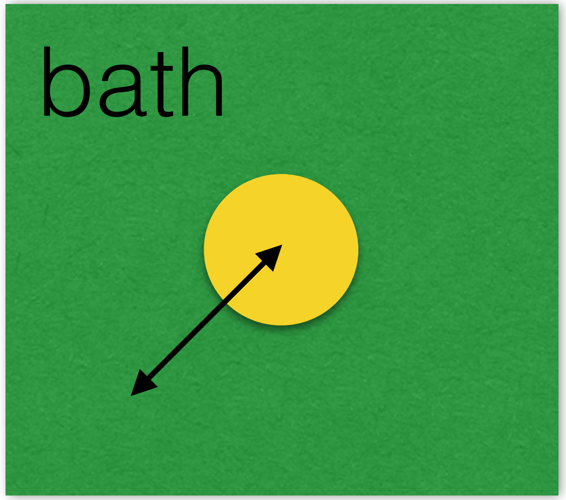
# Imaginary time Green's function

Alex Taekyung Lee

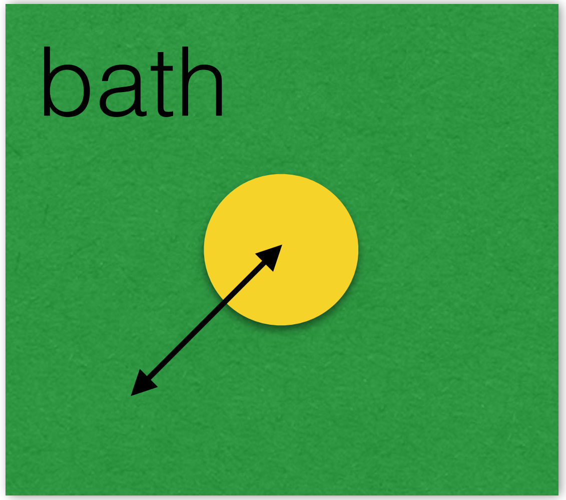
# Nonzero temperature

- 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 know, 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 know, since they are fluctuating between different configurations.




- All we know: temperature = mean energy
- => Green's function should be averaged

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

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 => **τ**:

$$\begin{aligned} A(\tau) &= e^{\tau H} A e^{-\tau H}, \qquad \text{Heisenberg} \\ A_I(\tau) &= e^{\tau H_0} A e^{-\tau H_0}, \qquad \text{Interaction} \end{aligned}$$

$$\begin{aligned} U_I(\tau, \tau') &= e^{\tau H_0} e^{-(\tau-\tau')H} e^{-\tau' H_0} = T_\tau \exp(-\int_{\tau'}^{\tau} d\tau_1 V_I(\tau_1)) \\ e^{-\beta H} &= e^{-\beta H_0} U_I(\beta, 0) = e^{-\beta H_0} T_\tau \exp(-\int_0^{\beta} d\tau_1 V_I(\tau_1)) \end{aligned}$$

# Imaginary time and Matsubara green's function

- From the real-time heisenberg picture: $A(t) = e^{itH} A e^{-itH}$
- Replace it => **τ**:
$$\begin{aligned} A(\tau) &= e^{\tau H} A e^{-\tau H}, && \text{Heisenberg} \\ A_I(\tau) &= e^{\tau H_0} A e^{-\tau H_0}, && \text{Interaction} \end{aligned}$$
- **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:

$$T_\tau \left(A(\tau) B(\tau')\right) = \theta(\tau - \tau') A(\tau) B(\tau') \pm \theta\left(\tau' - \tau\right) B(\tau') A(\tau), \quad \begin{cases} + \text{ for bosons,} \\ - \text{ for fermions.} \end{cases}$$

# Properties of Matsubara green's function

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

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

$$\begin{aligned} C_{AB}(\tau,\tau') &= \frac{-1}{Z}\mathrm{Tr}[e^{-\beta H}e^{\tau H}Ae^{-\tau H}e^{\tau' H}Be^{-\tau' H}] \\ &= \frac{-1}{Z}\mathrm{Tr}[e^{-\beta H}e^{(\tau-\tau')H}Ae^{-(\tau-\tau')H}B] = C_{AB}(\tau-\tau') \ \text{ for } \tau > \tau'. \end{aligned}$$

# Properties of Matsubara green's function

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

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

$$\begin{aligned} C_{AB}(\tau,\tau') &= \frac{-1}{Z}\mathrm{Tr}[e^{-\beta H}e^{\tau H}Ae^{-\tau H}e^{\tau' H}Be^{-\tau' H}] \\ &= \frac{-1}{Z}\mathrm{Tr}[e^{-\beta H}e^{(\tau-\tau')H}Ae^{-(\tau-\tau')H}B] = C_{AB}(\tau-\tau') \ \text{ for } \tau > \tau'. \end{aligned}$$

2. $C_{AB}(\boldsymbol{\tau}-\boldsymbol{\tau}')$ is naturally defined in the interval of $-\beta < \boldsymbol{\tau}-\boldsymbol{\tau}' < \beta$.

Otherwise it diverges. It is clear if we consider Lehman representation for $\boldsymbol{\tau} > \boldsymbol{\tau}'$

$$C_{AB}(\tau-\tau') = \frac{-1}{Z}\sum_{n,n'}[e^{-\beta E_n}e^{(\tau-\tau')E_n}A_{nn'}e^{-(\tau-\tau')E_{n'}}B_{n'n}]$$

# Properties of Matsubara green's function

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

+: boson
−: fermion

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

$$
\begin{aligned}
C_{AB}(\tau) &= \pm \frac{-1}{Z}\mathrm{Tr}[e^{-\beta H} B e^{\tau H} A e^{-\tau H}] = \pm \frac{-1}{Z}\mathrm{Tr}[e^{\tau H} A e^{-(\beta+\tau)H} B] \\
&= \pm \frac{-1}{Z}\mathrm{Tr}[e^{-\beta H} e^{(\tau+\beta)H} A e^{-(\beta+\tau)H} B] = \pm C_{AB}(\tau+\beta).
\end{aligned}
$$

# Properties of Matsubara green's function

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

+: boson
−: fermion

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

$$
\begin{aligned}
C_{AB}(\tau) &= \pm \frac{-1}{Z} \mathrm{Tr}[e^{-\beta H} B e^{\tau H} A e^{-\tau H}] = \pm \frac{-1}{Z} \mathrm{Tr}[e^{\tau H} A e^{-(\beta+\tau)H} B] \\
&= \pm \frac{-1}{Z} \mathrm{Tr}[e^{-\beta H} e^{(\tau+\beta)H} A e^{-(\beta+\tau)H} B] = \pm C_{AB}(\tau + \beta).
\end{aligned}
$$

**Using imaginary time**

**=> we can treat temperature as time!**

# Fourier transform of Matsubara green's function

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

$$\mathcal{C}_{AB}(n) \equiv \frac{1}{2}\int_{-\beta}^{\beta} d\tau\, e^{i\pi n\tau/\beta}\mathcal{C}_{AB}(\tau),$$

$$\mathcal{C}_{AB}(\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\pi n\tau/\beta}\mathcal{C}_{AB}(n).$$

- They become

$$\mathcal{C}_{AB}(n) = \int_{0}^{\beta} d\tau\, e^{i\pi n\tau/\beta}\mathcal{C}_{AB}(\tau), \quad \begin{cases} n \text{ is even for bosons,} \\ n \text{ is odd for fermions.} \end{cases}$$

$$\mathcal{C}_{AB}(i\omega_n) = \int_{0}^{\beta} d\tau\, e^{i\omega_n\tau}\mathcal{C}_{AB}(\tau), \quad \begin{cases} \omega_n = \frac{2n\pi}{\beta}, & \text{for bosons,} \\ \omega_n = \frac{(2n+1)\pi}{\beta}, & \text{for fermions.} \end{cases}$$

- $\omega_n$ is called as Matsubara frequency

# Example: non interacting particle

- Single particle Matsubara Green's function:

$$\mathcal{G}(\mathbf{r}\sigma\tau,\mathbf{r}'\sigma\tau') = -\left\langle T_\tau\left(\Psi_\sigma(\mathbf{r},\tau)\Psi_\sigma^\dagger(\mathbf{r}',\tau')\right)\right\rangle, \quad \text{real space},$$

$$\mathcal{G}(\nu\tau,\nu'\tau') = -\left\langle T_\tau\left(c_\nu(\tau)c_{\nu'}^\dagger(\tau')\right)\right\rangle, \quad \{\nu\} \text{ representation}.$$

- Consider a Hamiltonian: $H_0 = \sum_\nu \xi_\nu c_\nu^\dagger c_\nu,$

# Example: non interacting particle

- Single particle Matsubara Green's function:

$$\mathcal{G}(\mathbf{r}\sigma\tau, \mathbf{r}'\sigma\tau') = -\left\langle T_\tau \left( \Psi_\sigma(\mathbf{r},\tau)\Psi_\sigma^\dagger(\mathbf{r}',\tau') \right) \right\rangle, \quad \text{real space},$$

$$\mathcal{G}(\nu\tau, \nu'\tau') = -\left\langle T_\tau \left( c_\nu(\tau) c_{\nu'}^\dagger(\tau') \right) \right\rangle, \quad \{\nu\} \text{ representation}.$$

- Consider a Hamiltonian: $H_0 = \sum_\nu \xi_\nu c_\nu^\dagger c_\nu,$

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

# Example: non interacting particle

- Single particle Matsubara Green's function:

$$\mathcal{G}(\mathbf{r}\sigma\tau, \mathbf{r}'\sigma\tau') = -\left\langle T_\tau \left( \Psi_\sigma(\mathbf{r},\tau)\Psi^\dagger_\sigma(\mathbf{r}',\tau') \right) \right\rangle, \quad \text{real space,}$$

$$\mathcal{G}(\nu\tau, \nu'\tau') = -\left\langle T_\tau \left( c_\nu(\tau) c^\dagger_{\nu'}(\tau') \right) \right\rangle, \quad \{\nu\} \text{ representation.}$$

- Consider a Hamiltonian: $H_0 = \sum_\nu \xi_\nu c^\dagger_\nu c_\nu,$

$$c_\nu(\tau) = e^{\tau H_0} c_\nu e^{-\tau H_0} = e^{-\xi_\nu \tau} c_\nu, \qquad c^\dagger_\nu(\tau) = e^{\tau H_0} c^\dagger_\nu e^{-\tau H_0} = e^{\xi_\nu \tau} c^\dagger_\nu,$$

$$\begin{aligned}
\mathcal{G}_0(\nu, \tau - \tau') &= -\left\langle T_\tau \left( c_\nu(\tau) c^\dagger_\nu(\tau') \right) \right\rangle, \\
&= -\theta(\tau - \tau')\langle c_\nu(\tau) c^\dagger_\nu(\tau')\rangle - (\pm)\,\theta(\tau' - \tau)\langle c^\dagger_\nu(\tau') c_\nu(\tau)\rangle \\
&= -\left[ \theta(\tau - \tau')\langle c_\nu c^\dagger_\nu\rangle (\pm) \theta(\tau' - \tau)\langle c^\dagger_\nu c_\nu\rangle \right] e^{-\xi_\nu(\tau - \tau')},
\end{aligned}$$

# Example: non interacting particle

- For fermion:

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

$$\mathcal{G}_{0,F}(\nu, ik_n) = \int_0^\beta d\tau \, e^{ik_n \tau} \mathcal{G}_{0,F}(\nu, \tau), \quad k_n = (2n+1)\,\pi/\beta$$

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

$$n_F = < c_\nu^\dagger c_\nu > = \frac{1}{e^{\beta\xi} + 1}$$

# Example: non interacting particle

- For fermion:

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

$$\mathcal{G}_{0,F}(\nu,ik_n) = \int_0^\beta d\tau\, e^{ik_n\tau}\mathcal{G}_{0,F}(\nu,\tau), \quad k_n = (2n+1)\,\pi/\beta$$

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

$$n_F = < c_\nu^\dagger c_\nu > = \frac{1}{e^{\beta\xi}+1}$$

- For boson:

$$\mathcal{G}_{0,B}(\nu,\tau-\tau') = -\left[\theta(\tau-\tau')\,(1+n_B(\xi_\nu)) + \theta(\tau'-\tau)n_B(\xi_\nu)\right] e^{-\xi_\nu(\tau-\tau')}$$

$$\mathcal{G}_{0,B}(\nu,iq_n) = \int_0^\beta d\tau\, e^{iq_n\tau}\mathcal{G}_{0,B}(\nu,\tau), \quad q_n = 2n\pi/\beta$$

$$= \frac{1}{iq_n - \xi_\nu}$$

# 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:

$$G_0(\nu, i\omega_n \to \omega + i\eta) \;=\; \frac{1}{\omega - \xi_\nu + i\eta} = G_0^R(\omega)$$

# 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:

$$G_0(\nu, i\omega_n \to \omega + i\eta) = \frac{1}{\omega - \xi_\nu + i\eta} = G_0^R(\omega)$$

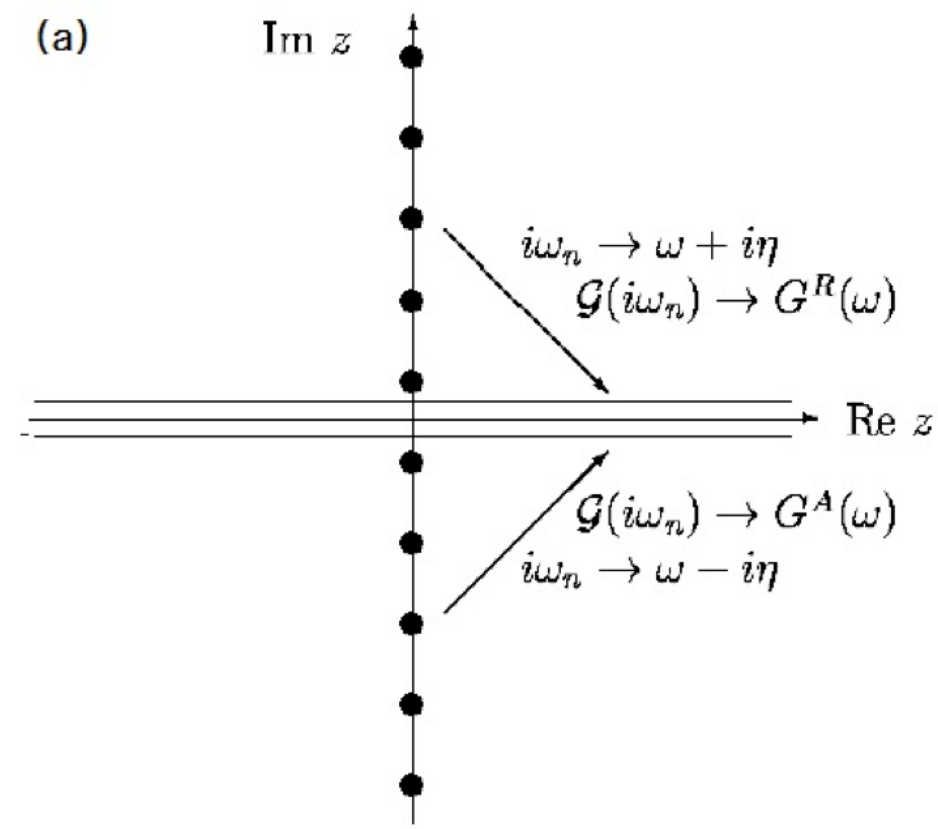



Figure from Bruus and Flensberg

# Reference

- Many-Particle Physics, Mahan
- Many-Body Quantum Theory in Condensed Matter Physics, Bruus and Flensberg

# Appendix

# Interaction picture

$$\text{The Schrödinger picture} \begin{cases} \text{states}: & |\psi(t)\rangle = e^{-iHt}\,|\psi_0\rangle, \\ \text{operators}: & A, \;\; \text{may or may not depend on time.} \\ & H, \;\; \text{does not depend on time.} \end{cases}$$

# Interaction picture

The Schrödinger picture

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

The Heisenberg picture

$$\begin{cases} \text{states :} & |\psi_0\rangle \equiv e^{iHt}\,|\psi(t)\rangle, \\ \text{operators :} & A(t) \equiv e^{iHt} A\, e^{-iHt}. \\ & H \quad \text{does not depend on time.} \end{cases}$$

# Interaction picture

$$\text{The Schrödinger picture} \begin{cases} \text{states}: & |\psi(t)\rangle = e^{-iHt}\,|\psi_0\rangle, \\ \text{operators}: & A, \;\text{ may or may not depend on time.} \\ & H, \;\text{ does not depend on time.} \end{cases}$$

$$\text{The Heisenberg picture} \begin{cases} \text{states}: & |\psi_0\rangle \;\equiv\; e^{iHt}\,|\psi(t)\rangle, \\ \text{operators}: & A(t) \;\equiv\; e^{iHt}A\,e^{-iHt}. \\ & H \quad \text{does not depend on time.} \end{cases}$$

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

$$\text{The interaction picture} \begin{cases} \text{states}: & |\hat{\psi}(t)\rangle \;\equiv\; e^{iH_0t}\,|\psi(t)\rangle, \\ \text{operators}: & \hat{A}(t) \;\equiv\; e^{iH_0t}A\,e^{-iH_0t}. \\ & H_0 \quad \text{does not depend on time.} \end{cases}$$

$$|\hat{\psi}(t)\rangle = \hat{U}(t,t_0)\,|\hat{\psi}(t_0)\rangle$$

U: unitary

# Imaginary time (1)

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

- Replace it => **τ**: 
$$A(\tau) = e^{\tau H} A e^{-\tau H}, \quad \text{Heisenberg}$$
$$A_I(\tau) = e^{\tau H_0} A e^{-\tau H_0}, \quad \text{Interaction}$$

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

- The thermal average is written, in terms of $U_I(\tau,\tau')$:

$$e^{-\beta H} = e^{-\beta H_0} U_I(\beta, 0) = e^{-\beta H_0} T_\tau \exp(-\int_0^\beta d\tau_1 V_I(\tau_1))$$

# Imaginary time (2)

- For example, consider the averaged correlation function with imaginary time:

$$\begin{aligned}\langle T_\tau A(\tau)B(\tau')\rangle &= \frac{1}{Z}\mathrm{Tr}\{e^{-\beta H}T_\tau[A(\tau)B(\tau')]\} \\ &= \frac{1}{Z}\mathrm{Tr}[e^{-\beta H_0}T_\tau(U_I(\beta,0)A_I(\tau)B_I(\tau'))] \\ &= \frac{\langle T_\tau(U_I(\beta,0)A_I(\tau)B_I(\tau'))\rangle_0}{\langle U_I(\beta,0)\rangle_0}\end{aligned}$$

- where we have:

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

$$Z_0 = \mathrm{Tr}e^{-\beta H_0}$$

# Fourier transform of Matsubara green's function

$$
\begin{aligned}
\mathcal{C}_{AB}(n) &= \frac{1}{2}\int_0^\beta d\tau\, e^{i\pi n\tau/\beta}\mathcal{C}_{AB}(\tau) + \frac{1}{2}\int_{-\beta}^0 d\tau\, e^{i\pi n\tau/\beta}\mathcal{C}_{AB}(\tau),\\
&= \frac{1}{2}\int_0^\beta d\tau\, e^{i\pi n\tau/\beta}\mathcal{C}_{AB}(\tau) + e^{-i\pi n}\frac{1}{2}\int_0^\beta d\tau\, e^{i\pi n\tau/\beta}\mathcal{C}_{AB}(\tau-\beta),\\
&= \frac{1}{2}\left(1 \pm e^{-i\pi n}\right)\int_0^\beta d\tau\, e^{i\pi n\tau/\beta}\mathcal{C}_{AB}(\tau),
\end{aligned}
$$

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:

$$\begin{aligned}\mathcal{G}_{0,F}(\nu, ik_n) &= \int_0^\beta d\tau\, e^{ik_n\tau}\mathcal{G}_{0,F}(\nu,\tau), \quad k_n = (2n+1)\,\pi/\beta \\ &= -\left(1 - n_F(\xi_\nu)\right)\int_0^\beta d\tau\, e^{ik_n\tau}e^{-\xi_\nu\tau}, \\ &= -\left(1 - n_F(\xi_\nu)\right)\frac{1}{ik_n - \xi_\nu}\left(e^{ik_n\beta}e^{-\xi_\nu\beta} - 1\right), \\ &= \frac{1}{ik_n - \xi_\nu},\end{aligned}$$

because $e^{ik_n\beta} = -1$ and $1 - n_F(\varepsilon) = \left(e^{-\beta\varepsilon} + 1\right)^{-1}$

# Example: non interacting particle

- For boson:

$$
\begin{aligned}
\mathcal{G}_{0,B}(\nu, iq_n) &= \int_0^\beta d\tau\, e^{iq_n\tau} \mathcal{G}_{0,B}(\nu, \tau), \quad q_n = 2n\pi/\beta \\
&= -\left(1 + n_B(\xi_\nu)\right) \int_0^\beta d\tau\, e^{iq_n\tau} e^{-\xi_\nu \tau}, \\
&= -\left(1 + n_B(\xi_\nu)\right) \frac{1}{iq_n - \xi_\nu} \left(e^{iq_n\beta} e^{-\xi_\nu\beta} - 1\right) \\
&= \frac{1}{iq_n - \xi_\nu},
\end{aligned}
$$

using $e^{iq_n\beta} = 1 \text{ and } 1 + n_B(\varepsilon) = -\left(e^{-\beta\varepsilon} - 1\right)^{-1}.$

# Various Green's functions

1. **Retarded Green function**

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

2. **Advanced Green function**

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

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**

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

5. **Time-ordered Green function**

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