Quantum Theory of Many-Body systems in Condensed Matter (4302112) 2020

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Today's class: *Matsubara formalism – Imaginary-time GFs*

- Imaginary-time evolution of operators.
- Imaginary-time ordered Green's functions.
- Sum over Matsubara frequencies.
- Feynman diagrams for Matsubara Green's functions.

Imaginary time evolution

Correlation functions at finite temperatures.

$$\left\langle \hat{a}_k(t)\hat{a}^\dagger_{k'}(t')\right\rangle = \frac{1}{\mathcal{Z}}\mathrm{Tr}\,\left(e^{-\beta\hat{H}}e^{i\hat{H}t}\hat{a}_k e^{-i\hat{H}(t-t')}\hat{a}^\dagger_{k'}e^{-i\hat{H}t'}\right)$$

"Imaginary time"

$$t \to -i\tau \Rightarrow e^{-\beta\hat{H}}e^{i\hat{H}t} = e^{\hat{H}(\tau-\beta)}$$

$$\hat{A}_H(\tau) \equiv e^{\hat{H}\tau}\hat{A}e^{-\hat{H}\tau}$$

Heisenberg picture

Interaction picture :

$$\hat{U}(\tau,\tau_0) = e^{\hat{H}_0\tau}e^{-\hat{H}(\tau-\tau_0)}e^{-\hat{H}_0\tau_0}$$

$$\hat{A}_I(\tau) \equiv e^{\hat{H}_0\tau}\hat{A}e^{-\hat{H}_0\tau}$$

Interaction picture

Easy to show:

$$\begin{cases} \hat{A}_H(\tau) = \hat{U}(0,\tau)\hat{A}_I(\tau)\hat{U}(\tau,0) \\ e^{-\beta\hat{H}} = e^{-\beta\hat{H}_0}\hat{U}(\beta,0) \end{cases}$$

Matsubara Green's functions

$$\mathcal{G}_{\sigma\sigma'}(\vec{r},\tau;\vec{r}\,',\tau') = -\left\langle \mathcal{T}_\tau \left[\hat{\psi}_\sigma(\vec{r},\tau)\hat{\psi}^\dagger_{\sigma'}(\vec{r}\,',\tau')\right]\right\rangle$$

$$\mathcal{G}_{kk'}(\tau-\tau') = -\left\langle \mathcal{T}_\tau \left[\hat{a}_k(\tau)\hat{a}^\dagger_{k'}(\tau')\right]\right\rangle$$

Imaginary-time correlation functions

- Imaginary time ordering:

$$\mathcal{T}_\tau \left[\hat{a}_k(\tau)\hat{a}^\dagger_{k'}(\tau')\right] = \begin{cases} \hat{a}_k(\tau)\hat{a}^\dagger_{k'}(\tau') \text{ if } \tau > \tau' \\ \pm\hat{a}^\dagger_{k'}(\tau')\hat{a}_k(\tau) \text{ if } \tau' > \tau \end{cases}$$

+: Bosons -: Fermions

Free propagator.

$$\hat{H}_0 = \sum_k \epsilon_k \hat{a}^\dagger_k \hat{a}_k$$

[redacted]

$$\begin{cases} \mathcal{G}^{(0)}_{kk}(\tau-\tau') = -\left[\theta(\tau-\tau')\left(1 \pm n_{B(F)}(\epsilon_k,\beta)\right) \mp \theta(\tau'-\tau) n_{B(F)}(\epsilon_k,\beta)\right] e^{-\epsilon_k(\tau-\tau')} \\ \mathcal{G}^{(0)}_{kk}(i\omega_m) = \dfrac{1}{i\omega_m - \epsilon_k} \end{cases}$$

$$\Rightarrow e^{i\omega_m\beta} = \mp 1 \Rightarrow \omega_m = \begin{cases} 2m\pi/\beta & \text{Bosons} \\ (2m+1)\pi/\beta & \text{Fermions} \end{cases}$$

Interaction picture

Using $\hat{A}_H(\tau) = \hat{U}(0,\tau)\hat{A}_I(\tau)\hat{U}(\tau,0)$ and $e^{-\beta\hat{H}} = e^{-\beta\hat{H}_0}\hat{U}(\beta,0)$:

$$\mathcal{G}_{kk'}(\tau,\tau') = -\frac{\mathrm{Tr}\left\{e^{-\beta\hat{H}_0}U(\beta,\tau)(\hat{a}_k)_I(\tau)U(\tau,\tau')(\hat{a}^\dagger_{k'})_I(\tau')U(\tau',0)\right\}}{\mathrm{Tr}\left\{e^{-\beta\hat{H}_0}U(\beta,0)\right\}}$$

$$\mathcal{G}_{kk'}(\tau,\tau') = -\frac{\left\langle U(\beta,\tau)(\hat{a}_k)_I(\tau)U(\tau,\tau')(\hat{a}^\dagger_{k'})_I(\tau')U(\tau',0)\right\rangle_0}{\langle U(\beta,0)\rangle_0}$$

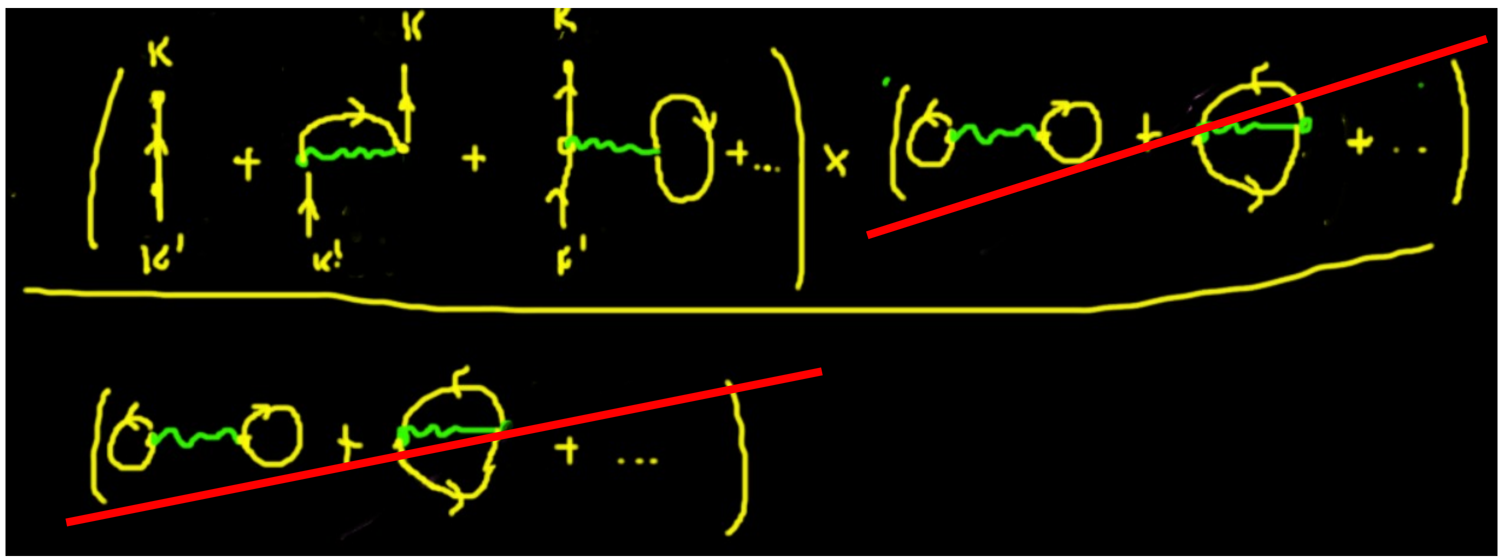
The thermal averages involve *non-interacting states* only!

Perturbative expansion: Feynman diagrams

Perturbative expansion in the interaction (quartic) term:

$$\mathcal{G}_{kk'}(\tau,\tau') = -\frac{\left\langle \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \ldots d\tau_n \mathcal{T}_\tau \left[\hat{H}_1(\tau_1) \ \ldots \hat{H}_1(\tau_n) (\hat{a}_k)_I(\tau) (\hat{a}_m^\dagger)_I(\tau') \right] \right\rangle_0}{\left\langle \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \ldots d\tau_n \mathcal{T}_\tau \left[\hat{H}_1(\tau_1) \ \ldots \hat{H}_1(\tau_n) \right] \right\rangle_0}$$

$$\begin{cases} \hat{H}_0 = \sum_k \epsilon_k \hat{a}_k^\dagger \hat{a}_k \\ \hat{H}_1 = \frac{1}{2} \sum_{\substack{km \\ k'm'}} V_{\substack{km \\ k'm'}} \hat{a}_k^\dagger \hat{a}_m^\dagger \hat{a}_{m'} \hat{a}_{k'} \end{cases}$$



Rules for Feynman diagrams

$$\mathcal{G}_{kk'}(\tau,\tau') = -\frac{\left\langle \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \ldots d\tau_n \mathcal{T}_\tau \left[\hat{H}_1(\tau_1)\ \ldots \hat{H}_1(\tau_n)(\hat{a}_k)_I(\tau)(\hat{a}_m^\dagger)_I(\tau')\right]\right\rangle_0}{\left\langle \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \ldots d\tau_n \mathcal{T}_\tau \left[\hat{H}_1(\tau_1)\ \ldots \hat{H}_1(\tau_n)\right]\right\rangle_0}$$

To evaluate the *n*-th order term in the expansion:

- Draw all connected, topologically distinct diagrams with *n* interaction lines beginning at (k',τ') and ending at (k,τ).
- Associate indices [(k',k''),(m',m''), etc.] to all interaction *2n* vertices.
- To every continuous line from (k_2, τ_2) → (k_1, τ_1) associate $\mathcal{G}^{(0)}_{k_1 k_2}(\tau_1,\tau_2)$
- To every interaction like, associate $-V_{\substack{k'm' \\ k''m''}}$
- Sum over internal indices and integrate over τ_n (=0 to β).
- Multiply each diagram by $(-1)^F$ where *F* =no. of fermionic closed loops.
- Multiply by $\frac{1}{n!}$

Rules for Feynman diagrams in (**k**,iω_m)

$$\mathcal{G}(\vec{k}, i\omega_m)$$

To evaluate the *n*-th order term in the expansion:

- Draw all connected, topologically distinct diagrams with *n* interaction lines.
- Associate (**k**$_i$,iω_{mi}) to propagating lines and (**q**,iq_n) to interaction lines.
- To every continuous line associate $\frac{1}{\beta V_{\mathbf{r}}}\mathcal{G}^{(0)}(\vec{k}_i, i\omega_{m_i})$
- To every interaction like, associate $-V(\vec{q}, iq_n)$ (i$q_n \rightarrow$ bosonic).
- To every equal time propagator associate $e^{i\omega_{m_i}\eta}$ with $\eta \rightarrow 0^+$
- Apply conservation of qadri-momenta (**k**$_i$,iω_{mi}) in each vertex.
- Integrate over internal momenta and sum over Matsubara frequencies.
- Multiply each diagram by $(-1)^F$ where *F* =no. of fermionic closed loops.
- Multiply by $\frac{1}{n!}$