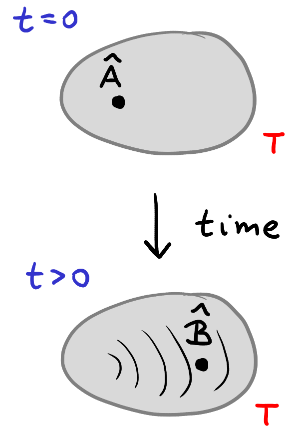
Thermal GFs & Matsubara representation

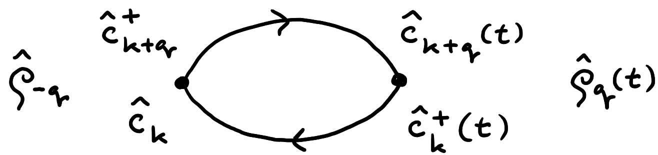


time evolution ~ quantum dynamics $\hat A(t) = e^{\frac{i}{\hbar}\hat H t}\,\hat A\, e^{-\frac{i}{\hbar}\hat H t}$

$$G_R(E) = -\frac{i}{\hbar}\int_{-\infty}^{\infty} \langle [\hat A(t), \hat B(0)]_\varepsilon \rangle\, e^{\frac{i}{\hbar}(E+i0^+)t}\, \vartheta(t)\, dt$$

thermal equilibrium ~ quantum statistics $\langle \hat O \rangle = \frac{1}{Z}\mathrm{Tr}\left(e^{-\beta \hat H}\hat O\right)$

- goal 1: unification of $e^{-\frac{i}{\hbar}\hat H t}$ and $e^{-\beta \hat H}$ → imaginary time and frequencies



product of two propagators ?

$$\langle \hat c^+_{k\sigma}(t)\, \hat c_{k\sigma} \rangle \langle \hat c_{k+q\sigma}(t)\, \hat c^+_{k+q\sigma} \rangle$$
$$- \langle \hat c_{k\sigma}\, \hat c^+_{k\sigma}(t) \rangle \langle \hat c^+_{k+q\sigma}\, \hat c_{k+q\sigma}(t) \rangle$$

- goal 2: systematic decomposition into simple propagators → time ordering & Wick

① Thermal GF – definition & properties

- definition $\mathcal{G}(\tau,\tau') = -\frac{1}{\hbar}\langle T\{\hat{A}(-i\tau)\hat{B}(-i\tau')\}\rangle$ (double-time thermal GF)

imaginary-time Heisenberg operators

$$\hat{A}(-i\tau) = e^{\frac{i}{\hbar}\hat{H}(-i\tau)}\,\hat{A}\,e^{-\frac{i}{\hbar}\hat{H}(-i\tau)} = e^{\frac{\tau}{\hbar}\hat{H}}\,\hat{A}\,e^{-\frac{\tau}{\hbar}\hat{H}}$$

simplified notation: $\hat{A}(-i\tau) \rightarrow \hat{A}(\tau)$

time-ordering operator

$$T\{\hat{A}(\tau)\hat{B}(\tau')\} = \hat{A}(\tau)\hat{B}(\tau')\,\vartheta(\tau-\tau') - \varepsilon\,\hat{B}(\tau')\hat{A}(\tau)\,\vartheta(\tau'-\tau)$$

$\varepsilon = -1$ bosonic

$\varepsilon = +1$ fermionic

- homogeneity in time for stationary $\hat{H}$

use cyclic property of Tr & commutation with $e^{-\beta\hat{H}}$

$$\mathrm{Tr}\left[e^{-\beta\hat{H}}\hat{A}(\tau)\hat{B}(\tau')\right] = \mathrm{Tr}\left[e^{-\beta\hat{H}}\,e^{\frac{\tau}{\hbar}\hat{H}}\,\hat{A}\,e^{-\frac{\tau}{\hbar}\hat{H}}\,e^{\frac{\tau'}{\hbar}\hat{H}}\,\hat{B}\,e^{-\frac{\tau'}{\hbar}\hat{H}}\right]$$

$$= \mathrm{Tr}\left[e^{-\beta\hat{H}}\,e^{\frac{\tau-\tau'}{\hbar}\hat{H}}\,\hat{A}\,e^{-\frac{\tau-\tau'}{\hbar}\hat{H}}\,\hat{B}\right] = \mathrm{Tr}\left[e^{-\beta\hat{H}}\hat{A}(\tau-\tau')\,\hat{B}(0)\right]$$

- Final definition

$$\mathcal{G}(\tau) = -\frac{1}{\hbar}\langle T\{\hat{A}(\tau)\hat{B}(0)\}\rangle \quad \text{with} \quad \hat{A}(\tau) = e^{\frac{\tau}{\hbar}\hat{H}}\hat{A}\,e^{-\frac{\tau}{\hbar}\hat{H}} \qquad (\mathcal{G}(\tau,\tau') = \mathcal{G}(\tau-\tau'))$$

- spectral representation in τ-domain using eigenbasis $|n\rangle$: $\quad \hat{H}|n\rangle = E_n|n\rangle$

$$-\hbar\,\mathcal{G}(\tau) = \frac{1}{Z}\sum_m \langle m|e^{-\beta\hat{H}}\,T\{\hat{A}(\tau)\hat{B}(0)\}|m\rangle$$

insert $\hat{1} = \sum_n |n\rangle\langle n|$

$$= \frac{1}{Z}\sum_m \langle m|e^{-\beta\hat{H}}\left[e^{\frac{\tau}{\hbar}\hat{H}}\hat{A}\,e^{-\frac{\tau}{\hbar}\hat{H}}\hat{B}\,\vartheta(\tau) - \varepsilon\,\hat{B}\,e^{\frac{\tau}{\hbar}\hat{H}}\hat{A}\,e^{-\frac{\tau}{\hbar}\hat{H}}\vartheta(-\tau)\right]|m\rangle$$

relabel $m \leftrightarrow n$

$$= \frac{1}{Z}\sum_{mn} e^{-\beta E_m}\left[e^{\frac{\tau}{\hbar}(E_m-E_n)}\langle m|\hat{A}|n\rangle\langle n|\hat{B}|m\rangle\,\vartheta(\tau) - \varepsilon\,e^{\frac{\tau}{\hbar}(E_n-E_m)}\langle m|\hat{B}|n\rangle\langle n|\hat{A}|m\rangle\,\vartheta(-\tau)\right]$$

$$\mathcal{G}(\tau) = -\frac{1}{\hbar}\frac{1}{Z}\sum_{mn}\langle m|\hat{A}|n\rangle\langle n|\hat{B}|m\rangle\left[e^{-\beta E_m}\vartheta(\tau) - \varepsilon\,e^{-\beta E_n}\vartheta(-\tau)\right]e^{\frac{\tau}{\hbar}(E_m-E_n)}$$

spectral representation of $G_R(t)$

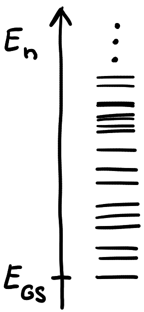
connection of $\mathcal{G}$ and G_R ?

$$G_R(t) = -\frac{i}{\hbar}\frac{1}{Z}\sum_{mn}\langle m|\hat{A}|n\rangle\langle n|\hat{B}|m\rangle\left(e^{-\beta E_m} + \varepsilon\,e^{-\beta E_n}\right)e^{\frac{i}{\hbar}(E_m-E_n)t}$$

- allowed τ range

$$\mathcal{G}(\tau) = -\frac{1}{\hbar}\frac{1}{Z}\sum_{mn} \langle m|\hat{A}|n\rangle\langle n|\hat{B}|m\rangle \left[e^{-\beta E_m}\,\vartheta(\tau) - \varepsilon\, e^{-\beta E_n}\,\vartheta(-\tau) \right] e^{\frac{\tau}{\hbar}(E_m - E_n)}$$

spectrum of $\hat{H}$ limited from the bottom by E_{GS} & typically unlimited at the top



$\tau > 0$: $\quad e^{-\beta E_m}\, e^{\frac{\tau}{\hbar}(E_m - E_n)} = e^{\left(\frac{\tau}{\hbar} - \beta\right)E_m}\, e^{-\frac{\tau}{\hbar}E_n}$

$\rightarrow \frac{\tau}{\hbar} - \beta \leq 0$ required since E_m may reach $+\infty$

$\tau < 0$: $\quad e^{-\beta E_n}\, e^{\frac{\tau}{\hbar}(E_m - E_n)} = e^{-\left(\frac{\tau}{\hbar} + \beta\right)E_n}\, e^{\frac{\tau}{\hbar}E_m}$

$\rightarrow \frac{\tau}{\hbar} + \beta \geq 0$ required

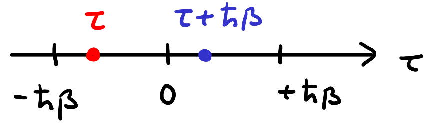
alltogether $\; -\hbar\beta \leq \tau \leq +\hbar\beta \;\rightarrow$ definition domain $\tau \in [-\hbar\beta, +\hbar\beta]$

($\mathcal{G}(\tau)$ typically exponentially explodes outside)

- symmetry of $\mathcal{G}$ with respect to τ-shift

$$\mathcal{G}(\tau) = -\frac{1}{\hbar}\frac{1}{Z}\sum_{mn}\langle m|\hat{A}|n\rangle\langle n|\hat{B}|m\rangle\left[e^{-\beta E_m}\vartheta(\tau) - \varepsilon\, e^{-\beta E_n}\vartheta(-\tau)\right] e^{\frac{\tau}{\hbar}(E_m-E_n)}$$

consider $\mathcal{G}(\tau<0)$ and $\mathcal{G}(\tau+\hbar\beta>0)$



$\tau<0$: $\quad e^{-\beta E_n}\, e^{\frac{\tau}{\hbar}(E_m-E_n)}$

$\tau+\hbar\beta>0$: $\quad e^{-\beta E_m}\, e^{(\frac{\tau}{\hbar}+\beta)(E_m-E_n)} = e^{-\beta E_n}\, e^{\frac{\tau}{\hbar}(E_m-E_n)}$

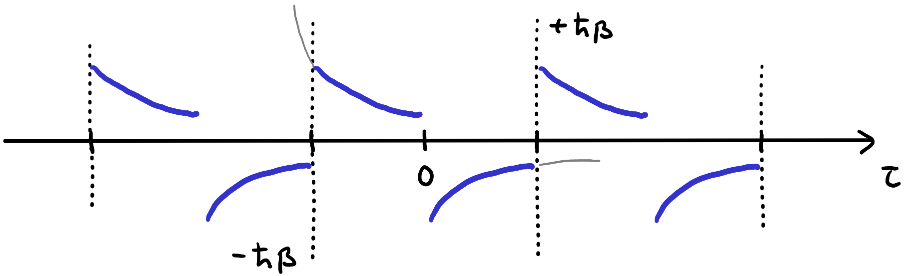
the same up to $-\varepsilon$ $\rightarrow$ conclusion: $\mathcal{G}(\tau) = -\varepsilon\,\mathcal{G}(\tau+\hbar\beta)$

alternative derivation using the cyclic property of trace:

$$\mathcal{G}(\tau+\hbar\beta>0) = -\frac{1}{\hbar Z}\mathrm{Tr}\Big[\underbrace{e^{-\beta\hat{H}}e^{(\frac{\tau}{\hbar}+\beta)\hat{H}}}_{e^{\frac{\tau}{\hbar}\hat{H}}}\hat{A}\,\underbrace{e^{-(\frac{\tau}{\hbar}+\beta)\hat{H}}}_{e^{-\frac{\tau}{\hbar}\hat{H}}e^{-\beta\hat{H}}}\hat{B}\Big] = -\frac{1}{\hbar Z}\mathrm{Tr}\Big[e^{-\beta\hat{H}}\hat{B}\,\underbrace{e^{\frac{\tau}{\hbar}}\hat{A}\,e^{-\frac{\tau}{\hbar}}}_{\hat{A}(\tau)}\Big] = \frac{\mathcal{G}(\tau<0)}{-\varepsilon}$$

(2) Matsubara representation

$G(\tau)$ periodically continued outside of $[-\hbar\beta, +\hbar\beta]$ and captured by Fourier series



period in τ : $2\hbar\beta$

$\downarrow$

possible frequencies :

$$\frac{2\pi}{\text{period}}\, n = \frac{\pi n}{\hbar\beta} \qquad n \in \mathbb{Z}$$

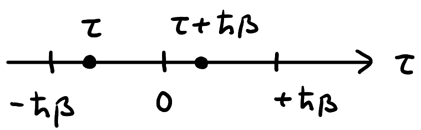
- Fourier series (coincides with thermal GF at $[-\hbar\beta, +\hbar\beta]$)

$$G(\tau) = \frac{1}{\hbar\beta} \sum_n G(iE_n)\, e^{-iE_n \frac{\tau}{\hbar}}$$

Matsubara energies $E_n = \frac{\pi n}{\beta}$

Fourier coefficients with the physical dimension $\frac{1}{\text{energy}} \times$ dim. of $\hat{A}\,\hat{B}$

- subsets of E_n selected by τ-shift symmetry of $G(\tau)$



$$G(\tau + \hbar\beta) = -\varepsilon\, G(\tau)$$

keep only compatible Fourier components

check Fourier components $e^{-iE_n\frac{\tau}{\hbar}}$, $E_n = \frac{\pi n}{\beta}$ against $\mathcal{G}(\tau+\hbar\beta) = -\varepsilon\,\mathcal{G}(\tau)$:

$\hbar\beta$-shifted exponential $e^{iE_n\frac{\tau+\hbar\beta}{\hbar}} = e^{i\frac{\pi n}{\beta}\left(\frac{\tau}{\hbar}+\beta\right)} = e^{iE_n\frac{\tau}{\hbar}}\, e^{in\pi}$

1) bosonic case $\varepsilon = -1$

$e^{in\pi} = +1 \;\rightarrow\;$ n is even $\rightarrow$ bosonic Matsubara energies $i\nu_n = i\,\frac{\pi}{\beta}\,2n$

2) Fermionic case $\varepsilon = +1$ $\qquad n \in \mathbb{Z}$

$e^{in\pi} = -1 \;\rightarrow\;$ n is odd $\rightarrow$ Fermionic Matsubara energies $iE_n = i\,\frac{\pi}{\beta}\,(2n+1)$

- evaluation of Fourier coefficients

$$\mathcal{G}(iE_n) = \hbar\beta\,\frac{1}{2\hbar\beta}\int_{-\hbar\beta}^{+\hbar\beta}\mathcal{G}(\tau)\,e^{iE_n\frac{\tau}{\hbar}}\,d\tau = \frac{1}{2}\int_0^{\hbar\beta}\Big[\mathcal{G}(\tau)\,e^{iE_n\frac{\tau}{\hbar}} + \overbrace{\mathcal{G}(\tau-\hbar\beta)}^{-\varepsilon\,\mathcal{G}(\tau)}\,\overbrace{e^{iE_n\frac{\tau-\hbar\beta}{\hbar}}}^{-\varepsilon\, e^{iE_n\frac{\tau}{\hbar}}}\Big]\,d\tau$$

$$= \int_0^{\hbar\beta}\mathcal{G}(\tau)\,e^{iE_n\frac{\tau}{\hbar}}\,d\tau$$

(the proper set of iE_n needs to be used!)

- spectral representation

$$\mathcal{G}(\tau) = -\frac{1}{\hbar}\frac{1}{Z}\sum_{mn} \langle m|\hat{A}|n\rangle\langle n|\hat{B}|m\rangle \left[e^{-\beta E_m}\vartheta(\tau) - \varepsilon\, e^{-\beta E_n}\vartheta(-\tau)\right] e^{\frac{\tau}{\hbar}(E_m-E_n)}$$

$$\mathcal{G}(iE_\ell) = -\frac{1}{\hbar}\frac{1}{Z}\sum_{mn} \langle m|\hat{A}|n\rangle\langle n|\hat{B}|m\rangle\, e^{-\beta E_m} \int_0^{\hbar\beta} e^{\frac{\tau}{\hbar}(E_m-E_n)}\, e^{iE_\ell\frac{\tau}{\hbar}}\, d\tau$$

$$\text{integral} = \frac{\hbar}{E_m-E_n+iE_\ell}\left[e^{(E_m-E_n+iE_\ell)\beta} - 1\right] \quad \& \text{ use } \quad e^{iE_\ell\beta} = -\varepsilon$$

Matsubara coefficients
$$\mathcal{G}(iE_\ell) = \frac{1}{Z}\sum_{mn} \langle m|\hat{A}|n\rangle\langle n|\hat{B}|m\rangle \frac{e^{-\beta E_m} - \varepsilon\, e^{-\beta E_n}}{iE_\ell + E_m - E_n}$$

compare to the spectral representation of $G_R(E)$

$$G_R(E) = \frac{1}{Z}\sum_{mn} \langle m|\hat{A}|n\rangle\langle n|\hat{B}|m\rangle \frac{e^{-\beta E_m} - \varepsilon\, e^{-\beta E_n}}{E + i0^+ + E_m - E_n}$$

→ origin in the same object $G(z\in\mathbb{C})$

$\nearrow$ $G_R(E) = G(E+i0^+)$

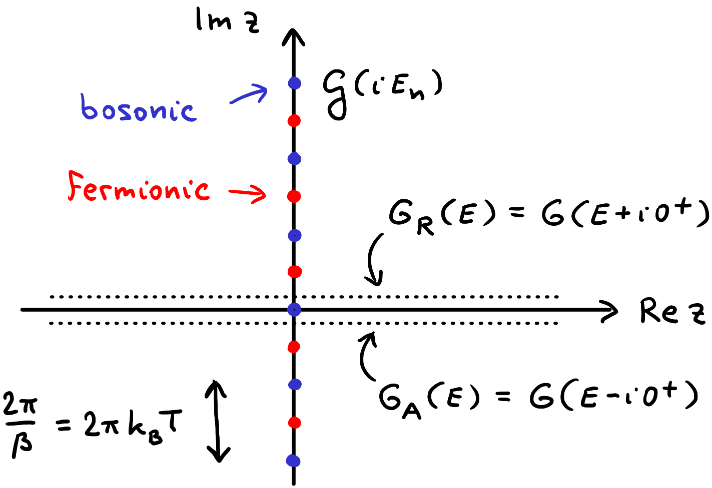
$\searrow$ $\mathcal{G}(iE_n) = G(iE_n)$

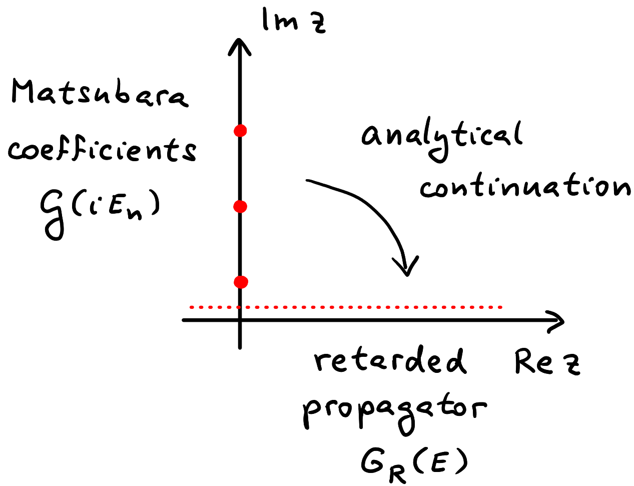
analytical continuation $iE_n \to E + i0^+$

- Mother of all propagators

$$G(z) = \frac{1}{Z} \sum_{mn} \langle m|\hat{A}|n\rangle \langle n|\hat{B}|m\rangle \, \frac{e^{-\beta E_m} - \varepsilon e^{-\beta E_n}}{z + E_m - E_n}$$

$G(z)$ has poles and branch cut on the real axis





Lehmann representation $\quad G(z) = \int_{-\infty}^{\infty} \frac{A(E)}{z - E} \, dE$

spectral function $\quad A(E) = \frac{1}{Z} \sum_{mn} \langle m|\hat{A}|n\rangle \langle n|\hat{B}|m\rangle \left(e^{-\beta E_m} + \varepsilon e^{-\beta E_n}\right) \delta[E - (E_n - E_m)]$

③ Single-particle GF for non-interacting electrons – Matsubara representation

- non-interacting electrons in a single band : $\hat{H} = \sum_{k\sigma} \varepsilon_k \hat{c}^+_{k\sigma} \hat{c}_{k\sigma}$ measured from μ

$$G(k,t) = -\frac{i}{\hbar} \langle \{ \hat{c}_k(t), \hat{c}^+_k(0) \} \rangle \vartheta(t) \longrightarrow G(k,z) = \frac{1}{z-\varepsilon_k} \quad \text{(lecture 3b)}$$

by analytical continuation $\quad \mathcal{G}(iE_n) = \dfrac{1}{iE_n - \varepsilon_k}$ at fermionic $iE_n = i\frac{\pi}{\beta}(2n+1)$

- direct evaluation using operator EOM for $\hat{c}_k(t)$ (EOM = equation of motion)

τ-domain analog of operator EOM $\dfrac{d\hat{A}}{dt} = \dfrac{1}{i\hbar}[\hat{A},\hat{H}]$:

$$\frac{d\hat{A}(\tau)}{d\tau} = \frac{d}{d\tau}\left(e^{\frac{\tau}{\hbar}\hat{H}} \hat{A} e^{-\frac{\tau}{\hbar}\hat{H}}\right) = e^{\frac{\tau}{\hbar}\hat{H}} \frac{1}{\hbar}\hat{H} \hat{A} e^{-\frac{\tau}{\hbar}\hat{H}} - e^{\frac{\tau}{\hbar}\hat{H}} \hat{A} \frac{1}{\hbar}\hat{H} e^{-\frac{\tau}{\hbar}\hat{H}} = -\frac{1}{\hbar}[\hat{A},\hat{H}]_\tau$$

$$[\hat{c}_{k\sigma}, \sum_{k'\sigma'} \varepsilon_k \hat{c}^+_{k'\sigma'} \hat{c}_{k'\sigma'}] = \varepsilon_k \Big(\underbrace{\hat{c}_{k\sigma} \hat{c}^+_{k\sigma} \hat{c}_{k\sigma}}_{\hat{c}_{k\sigma}} - \hat{c}^+_{k\sigma} \underbrace{\hat{c}_{k\sigma} \hat{c}_{k\sigma}}_{0} \Big) = \varepsilon_k \hat{c}_{k\sigma}$$

$$\frac{d\hat{c}_{k\sigma}(\tau)}{d\tau} = -\frac{1}{\hbar}\varepsilon_k \hat{c}_{k\sigma}(\tau) \rightarrow \hat{c}_{k\sigma}(\tau) = e^{-\frac{\tau}{\hbar}\varepsilon_k}\hat{c}_{k\sigma} \qquad \text{compare} \quad \hat{c}_{k\sigma}(t) = e^{-\frac{i}{\hbar}\varepsilon_k t}\hat{c}_{k\sigma}$$

propagator

$$g(k,\tau) = -\frac{1}{\hbar}\langle T\{\hat{c}_k(\tau)\hat{c}_k^+(0)\}\rangle = -\frac{1}{\hbar}\left[\langle \hat{c}_k(\tau)\hat{c}_k^+\rangle \vartheta(\tau) - \langle \hat{c}_k^+\hat{c}_k(\tau)\rangle \vartheta(-\tau)\right]$$

$$= -\frac{1}{\hbar}e^{-\frac{\tau}{\hbar}\varepsilon_k}\left[\underbrace{\langle \hat{c}_k\hat{c}_k^+\rangle}_{1-\langle c_k^+ c_k\rangle = 1-n_F(\varepsilon_k)}\vartheta(\tau) - \underbrace{\langle \hat{c}_k^+\hat{c}_k\rangle}_{n_F(\varepsilon_k)}\vartheta(-\tau)\right] = -\frac{1}{\hbar}e^{-\frac{\tau}{\hbar}\varepsilon_k}\left[\vartheta(\tau) - n_F(\varepsilon_k)\right]$$

Matsubara coefficients

$$g(k,iE_n) = \int_0^{\hbar\beta} d\tau\, g(k,\tau)\, e^{iE_n\frac{\tau}{\hbar}} = -\frac{1}{\hbar}\left[1-n_F(\varepsilon_k)\right]\int_0^{\hbar\beta} d\tau\, e^{-\frac{\tau}{\hbar}\varepsilon_k} e^{iE_n\frac{\tau}{\hbar}} = \left[1-n_F(\varepsilon_k)\right]\frac{-\left[e^{(iE_n-\varepsilon_k)\frac{\tau}{\hbar}}\right]_0^{\hbar\beta}}{\hbar\,\frac{iE_n-\varepsilon_k}{\hbar}}$$

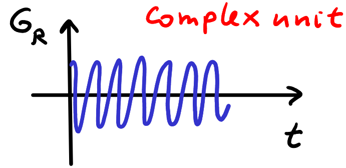
$$1-n_F(\varepsilon_k) = 1 - \frac{1}{e^{\beta\varepsilon_k}+1} = \frac{e^{\beta\varepsilon_k}}{e^{\beta\varepsilon_k}+1} = \frac{1}{1+e^{-\beta\varepsilon_k}}$$

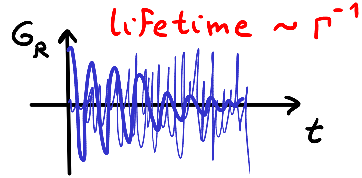
$$\left[e^{(iE_n-\varepsilon_k)\frac{\tau}{\hbar}}\right]_0^{\hbar\beta} = e^{iE_n\beta}e^{-\varepsilon_k\beta} - 1 = -e^{-\beta\varepsilon_k} - 1$$

$$\Bigg\} -1 \qquad = \frac{1}{iE_n - \varepsilon_k}$$

- Comparison of various forms of the single-electron propagator

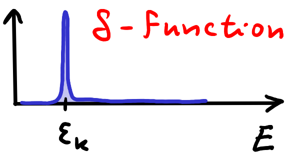
$$G_R(k,t) = -\frac{i}{\hbar}\, e^{-\frac{i}{\hbar}\varepsilon_k t}\, \vartheta(t)$$

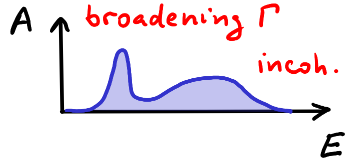




$$G_R(k,E) = \frac{1}{E - \varepsilon_k + i0^+}$$

$$A = -\frac{1}{\pi}\,\mathrm{Im}\, G_R$$

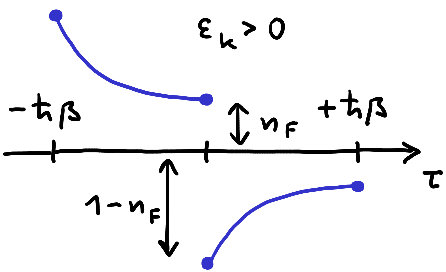


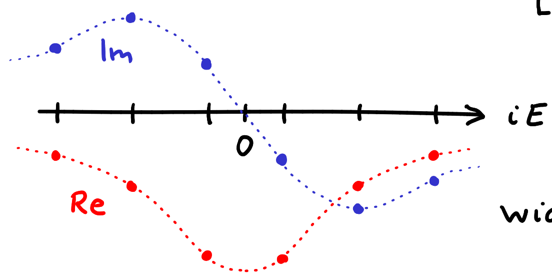


$$\mathcal{G}(k,\tau) = -\frac{1}{\hbar}\, e^{-\frac{1}{\hbar}\varepsilon_k \tau}\left[\vartheta(\tau) - n_F(\varepsilon_k)\right]$$

$$\mathcal{G}(k,iE_n) = \frac{1}{iE_n - \varepsilon_k} = \frac{-\varepsilon_k - iE_n}{\varepsilon_k^2 + E_n^2}$$

$E_n^2 = [\pi k_B T(2n+1)]^2$





width $\sim \varepsilon_k$

difficulties in analytical continuation if performed numerically

4 Lindhard Function via Matsubara Formalism

- density-density correlation function

$$\Pi_0(q,t) = V\frac{i}{\hbar}\langle[\hat{n}_q(t),\hat{n}_{-q}(0)]\rangle\vartheta(t) \qquad \Pi_0(q,\omega) = \int_{-\infty}^{\infty} dt\, e^{i(\omega+i0^+)t}\,\Pi_0(q,t)$$

thermal counterpart

$$\Pi_0(q,\tau) = V\frac{1}{\hbar}\langle T\{\hat{n}_q(\tau)\,\hat{n}_{-q}(0)\}\rangle \qquad \hat{n}_q = \frac{1}{V}\sum_{k\sigma}\hat{c}^\dagger_{k\sigma}\,\hat{c}_{k+q\sigma}$$

$$= \frac{1}{V}\frac{1}{\hbar}\sum_{k\sigma}\sum_{k'\sigma'}\langle T\{\hat{c}^\dagger_{k\sigma}(\tau^+)\,\hat{c}_{k+q\sigma}(\tau)\;\hat{c}^\dagger_{k'\sigma'}(0^+)\,\hat{c}_{k'-q\sigma'}(0)\}\rangle$$

infinitesimals added to keep $c^\dagger c$ order

- average of time-ordered string of creation/annihilation operators of non-interacting particles $\rightarrow$ sum of products of single-particle propagators

$$\langle T\{\hat{c}^\dagger_{k\sigma}(\tau^+)\,\hat{c}_{k+q\sigma}(\tau)\}\rangle\langle T\{\hat{c}^\dagger_{k'\sigma'}(0^+)\,\hat{c}_{k'-q\sigma'}(0)\}\rangle$$

$$-\langle T\{\hat{c}_{k+q\sigma}(\tau)\,\hat{c}^\dagger_{k'\sigma'}(0^+)\}\rangle\langle T\{\hat{c}_{k'-q\sigma'}(0)\,\hat{c}^\dagger_{k\sigma}(\tau)\}\rangle$$

T = 0 Wick 1950

T > 0 Matsubara 1955

Wick's theorem for averages (c is either $\hat{c}$ or $\hat{c}^+$)

$$\langle T\{c(t_1)\, c(t_2)\, c(t_3) \cdots c(t_N)\}\rangle_0 = \text{all possible pairwise pairings}$$

$$= \langle T\{c(t_1)c(t_2)\}\rangle_0 \langle T\{c(t_3)c(t_4)\rangle_0 \cdots \quad + \text{ other pairings}$$

example $\langle T\{c_1^+ c_2 c_3^+ c_4\}\rangle_0 =$

$+\langle T\{c_1^+ c_2\}\rangle_0 \langle T\{c_3^+ c_4\}\rangle_0$ 4 averages

$-\langle T\{c_1^+ c_3^+\}\rangle_0 \langle T\{c_2 c_4\}\rangle_0$ 4 averages $\rightarrow 0$

$+\langle T\{c_1^+ c_4\}\rangle_0 \langle T\{c_2 c_3^+\}\rangle_0$ 4 averages

in general: n creation ops & n annihilation ops $\rightarrow$ n! pairings

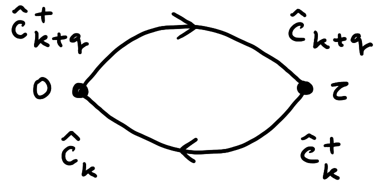
$$\langle T\{\hat{c}^+_{k\sigma}(\tau^+)\, \hat{c}_{k+q\sigma}(\tau)\, \hat{c}^+_{k'\sigma'}(0^+)\, \hat{c}_{k'-q\sigma'}(0)\}\rangle =$$

$$= \langle T\{\hat{c}^+_{k\sigma}(\tau^+)\, \hat{c}_{k+q\sigma}(\tau)\}\rangle \langle T\{\hat{c}_{k'\sigma'}(0^+)\, \hat{c}_{k'-q\sigma'}(0)\}\rangle \qquad n_{k\sigma}\, n_{k'\sigma'}\, \delta_{q0}$$

$$- \underbrace{\langle T\{\hat{c}_{k+q\sigma}(\tau)\, \hat{c}^+_{k'\sigma'}(0^+)\}\rangle}_{-\hbar G(k+q,\tau)\,\delta_{k+q,k'}\,\delta_{\sigma\sigma'}} \underbrace{\langle T\{\hat{c}_{k'-q\sigma'}(0)\, \hat{c}^+_{k\sigma}(\tau^+)\}\rangle}_{-\hbar G(k,-\tau)\,\delta_{k'-q,k}\,\delta_{\sigma\sigma'}}$$

- intermediate result – τ-domain

$$\Pi_0(q,\tau) = -\frac{1}{V}\hbar \sum_{k\sigma} \mathcal{G}(k+q,\tau)\,\mathcal{G}(k,-\tau)$$



- Fourier components

$$\Pi_0(q,i\nu_m) = \int_0^{\hbar\beta} d\tau\, \Pi_0(q,\tau)\, e^{i\nu_m \frac{\tau}{\hbar}} \qquad \mathcal{G}(k+q,\tau) = \frac{1}{\hbar\beta}\sum_n \mathcal{G}(k+q,iE_n)\, e^{-iE_n\frac{\tau}{\hbar}}$$

$$= \int_0^{\hbar\beta} d\tau\, \frac{1}{V}\hbar\sum_{k\sigma}\left[\frac{1}{\hbar\beta}\sum_{n'}\mathcal{G}(k+q,iE_{n'})\, e^{-iE_{n'}\frac{\tau}{\hbar}}\right]\left[\frac{1}{\hbar\beta}\sum_n \mathcal{G}(k,iE_n)\, e^{iE_n\frac{\tau}{\hbar}}\right] e^{i\nu_m\frac{\tau}{\hbar}}$$

$$\int_0^{\hbar\beta} d\tau\, e^{i(E_n+\nu_m-E_{n'})\frac{\tau}{\hbar}} = \hbar\,\frac{e^{i(E_n+\nu_m-E_{n'})\beta}-1}{i(E_n-\nu_m-E_{n'})} = \hbar\beta \quad \text{for } E_{n'} = E_n+\nu_m$$

→ discrete convolution at Matsubara frequencies / energies

$$\Pi_0(q,i\nu_m) = -\frac{1}{V}\sum_{k\sigma}\frac{1}{\beta}\sum_n \mathcal{G}(k+q,iE_n+i\nu_m)\,\mathcal{G}(k,iE_n)$$

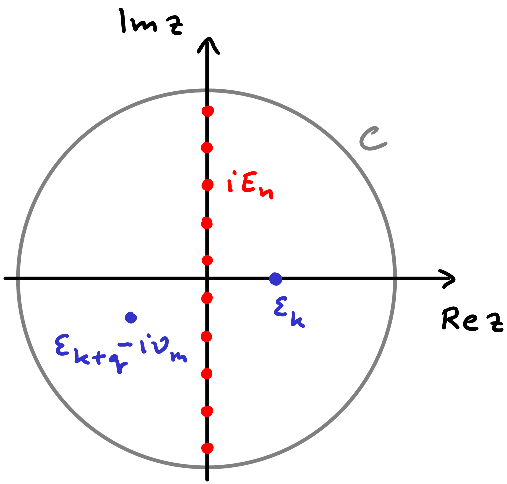
- evaluation of the convolution via contour integration

$$\Pi_0(q, i\nu_m) = -\frac{1}{V}\sum_{k\sigma}\frac{1}{\beta}\sum_n \mathcal{G}(k+q, iE_n + i\nu_m)\,\mathcal{G}(k, iE_n) = -\frac{1}{V}\sum_{k\sigma}\overbrace{\frac{1}{\beta}\sum_n \underbrace{\frac{1}{iE_n + i\nu_m - \varepsilon_{k+q}}\,\frac{1}{iE_n - \varepsilon_k}}_{f(z = iE_n)}}^{S}$$

observation:

$$n_F(z) = \frac{1}{e^{\beta z}+1} \quad \text{has poles at } \beta z = i\pi(2n+1) \rightarrow z_n = iE_n$$

expansion around poles z_n: $\quad e^{\beta(z-z_n)}e^{\beta z_n} + 1 \approx [1+\beta(z-z_n)](-1) + 1 = -\beta(z-z_n)$



$$f(z)\,n_F(z) = \frac{1}{z + i\nu_m - \varepsilon_{k+q}}\,\frac{1}{z - \varepsilon_k}\,n_F(z) \quad \text{has}$$

poles at $\varepsilon_{k+q} - i\nu_m$, ε_k, and $z_n = iE_n$

$f(z)\,n_F(z)$ vanishes at least as $\frac{1}{z^2}$ at $|z| \rightarrow \infty$

$$\oint_C dz\, f(z)\,n_F(z) = 0$$

$$= 2\pi i\left[\mathrm{Res}\,\varepsilon_k + \mathrm{Res}(\varepsilon_{k+q} - i\nu_m) + \sum_n \mathrm{Res}\,z_n\right]$$

$$f(z)\,n_F(z) = \frac{1}{z+i\nu_m-\varepsilon_{k+q}}\,\frac{1}{z-\varepsilon_k}\,n_F(z) \qquad n_F(z) \approx \frac{-1}{\beta(z-z_n)} \quad \text{around } z_n = iE_n$$

$$0 = \mathrm{Res}\,\varepsilon_k + \mathrm{Res}(\varepsilon_{k+q}-i\nu_m) + \sum_n \mathrm{Res}\,z_n = \frac{n_F(\varepsilon_{k+q}-i\nu_m)}{\varepsilon_{k+q}-i\nu_m-\varepsilon_k} + \frac{n_F(\varepsilon_k)}{\varepsilon_k+i\nu_m-\varepsilon_{k+q}} - \underbrace{\frac{1}{\beta}\sum_n f(iE_n)}_{S}$$

$$n_F(\varepsilon-i\nu_m) = \frac{1}{e^{\beta(\varepsilon-i\nu_m)}+1} = \frac{1}{e^{\beta\varepsilon}e^{\beta i\nu_m}+1} = n_F(\varepsilon)$$

$$e^{\beta i\nu_m} = e^{\beta i\frac{\pi}{\beta}2n} = 1$$

Final expression for the iE_n sum

$$S = \frac{1}{\beta}\sum_n \frac{1}{iE_n+i\nu_m-\varepsilon_{k+q}}\,\frac{1}{iE_n-\varepsilon_k} = \frac{n_F(\varepsilon_{k+q})-n_F(\varepsilon_k)}{\varepsilon_{k+q}-\varepsilon_k-i\nu_m}$$

Lindhard function in Matsubara representation

$$\Pi_0(q,i\nu_m) = -\frac{1}{V}\sum_{k\sigma}\frac{1}{\beta}\sum_n \frac{1}{iE_n+i\nu_m-\varepsilon_{k+q}}\,\frac{1}{iE_n-\varepsilon_k} = \frac{2}{V}\sum_k \frac{n_F(\varepsilon_k)-n_F(\varepsilon_{k+q})}{\varepsilon_{k+q}-\varepsilon_k-i\nu_m}$$

analytical continuation $i\nu_m \to \hbar\omega + i0^+$ gives the same formula as in lecture 5

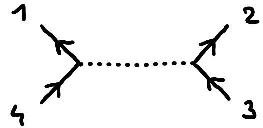
⑤ Why? Roadmap – systematic perturbation theory

- Dyson's formula

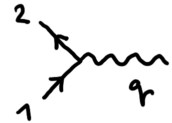
$$\hat{U}(\tau,\tau') = \sum_{n=0}^{\infty} \frac{1}{n!}\left(-\frac{1}{\hbar}\right)^n T\left\{ \int_{\tau'}^{\tau} d\tau_1 \int_{\tau'}^{\tau} d\tau_2 \cdots \int_{\tau'}^{\tau} d\tau_n \; \tilde{V}(\tau_1)\,\tilde{V}(\tau_2) \cdots \underset{\substack{\uparrow \\ \text{perturbation Hamiltonian}}}{\tilde{V}(\tau_n)} \right\}$$

- perturbations

Coulomb interaction $\quad H_{coul} = \frac{1}{2}\sum V_q\, c_1^+ c_2^+ c_3 c_4$

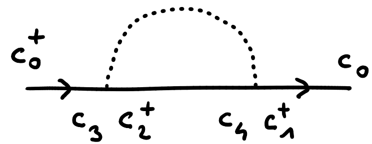


e-ph interaction $\quad H_{e\text{-}ph} = \sum M_{kq}(a_q + a_{-q}^+)\, c_1^+ c_2$



- Wick's theorem

$$\mathcal{G} = \langle T\{c_0 c_0^+\}\rangle + \langle T\{c_0 \;\sum V_q\, c_1^+ c_2^+ c_3 c_4 \;\; c_0^+\}\rangle + \ldots$$



τ- integrals of $\mathcal{G}_0(k,\tau) \xrightarrow{FT}$ convolutions of $\mathcal{G}_0(k, iE_n)$

- set of diagrams & translation rules $\longrightarrow \mathcal{G}(iE_n) \longrightarrow G_R(E)$