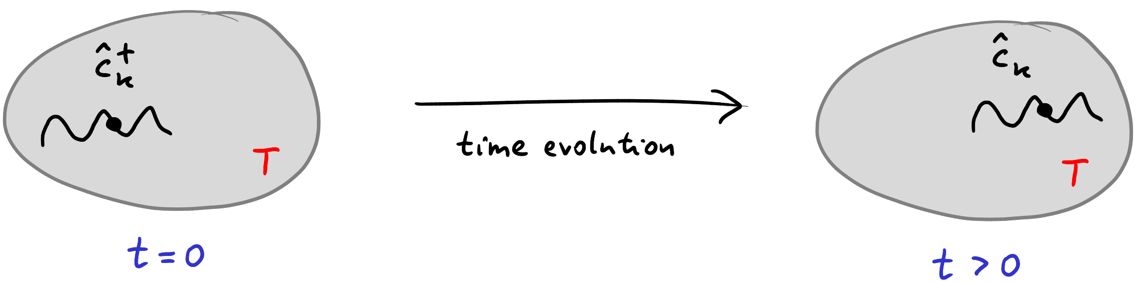
Propagators/Green's functions in many-body physics

- motivation – equilibrium electron propagator

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

$$G_{ret}(k,E) = -\frac{i}{\hbar}\int_{-\infty}^{\infty} \langle \{\hat{c}_k(t), \hat{c}_k^+(0)\} \rangle \, e^{\frac{i}{\hbar}(E+i0^+)t}\, \vartheta(t)\, dt$$

quantum statistics $\langle \hat{A} \rangle = \mathrm{Tr}(\hat{\rho}\hat{A}) = \frac{1}{Z}\sum_{\text{states}} \langle n | e^{-\beta\hat{H}}\hat{A} | n \rangle$



① Time evolution in Heisenberg picture

- time-evolution operator in case of time-independent $\hat{H}$

Schrödinger equation $i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$

using eigenbasis of $\hat{H}$ satisfying $\hat{H}|n\rangle = E_n|n\rangle$: $|\psi(t)\rangle = \sum_n c_n(t)|n\rangle$

$\rightarrow$ ODE for coefficients $i\hbar \frac{d}{dt} c_n = E_n c_n \rightarrow c_n(t) = e^{-\frac{i}{\hbar}E_n t} c_n(0)$

captured by $|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle$ since $e^{-\frac{i}{\hbar}\hat{H}t} = \sum_n e^{-\frac{i}{\hbar}E_n t}|n\rangle\langle n|$

time-evolution operator $\hat{U}(t,t') = e^{-\frac{i}{\hbar}\hat{H}(t-t')}$ acting as $|\psi(t)\rangle = \hat{U}(t,t')|\psi(t')\rangle$

- Schrödinger picture

$$\left.\begin{array}{lll} \text{1. evolve state vectors} & |\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle \\ \text{2. operators constant in time} & \hat{A} \end{array}\right\} \begin{array}{l} \text{averages} \\ \langle A\rangle_t = \langle\psi(t)|\hat{A}|\psi(t)\rangle \end{array}$$

- Heisenberg picture

time evolution of an average of an operator $\hat{A}$ decomposed differently

$$\langle A\rangle_t = \langle\Psi(t)|\hat{A}|\Psi(t)\rangle = \langle\Psi_{t=0}|\underbrace{e^{\frac{i}{\hbar}\hat{H}t}\hat{A}e^{-\frac{i}{\hbar}\hat{H}t}}_{\hat{A}(t)}|\Psi_{t=0}\rangle$$

1. state vectors constant $|\Psi\rangle = |\Psi_{t=0}\rangle$

2. operators evolve in time as $\hat{A}(t) = e^{\frac{i}{\hbar}\hat{H}t}\hat{A}e^{-\frac{i}{\hbar}\hat{H}t}$ note: $\hat{H}(t) = \hat{H}$

(interpretation – operator $\hat{A}$ applied at time t)

- Bloch equation

$$\frac{d}{dt}\hat{A}(t) = \frac{de^{\frac{i}{\hbar}\hat{H}t}}{dt}\hat{A}e^{-\frac{i}{\hbar}\hat{H}t} + e^{\frac{i}{\hbar}\hat{H}t}\hat{A}\frac{de^{-\frac{i}{\hbar}\hat{H}t}}{dt} = \frac{i}{\hbar}\hat{H}\hat{A}(t) + \hat{A}(t)\left(-\frac{i}{\hbar}\hat{H}\right)$$

$$= \frac{1}{i\hbar}[\hat{A}(t),\hat{H}]$$

$$= \frac{1}{i\hbar}[\hat{A},\hat{H}]_t$$

immediate consequence:

Ehrenfest theorem $\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle$

② Definition of equilibrium many-body propagators

- retarded double-time GF (the "physical" GF)

$$G_R(t,t') = -\frac{i}{\hbar}\langle [\hat{A}(t),\hat{B}(t')]_\varepsilon \rangle\, \vartheta(t-t')$$

commutator

$[\hat{A},\hat{B}]_\varepsilon = AB + \varepsilon BA$ — fermionic ops. $\hat{A},\hat{B}$: $\varepsilon = +1$ i.e. $[\hat{A},\hat{B}]_\varepsilon = \{\hat{A},\hat{B}\}$

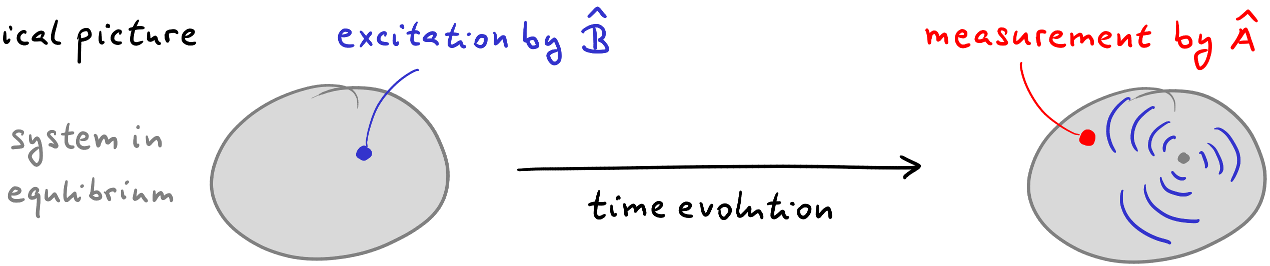
$[\hat{A},\hat{B}]_\varepsilon = AB + \varepsilon BA$ — bosonic ops. $\hat{A},\hat{B}$: $\varepsilon = -1$ i.e. $[\hat{A},\hat{B}]_\varepsilon = [\hat{A},\hat{B}]$

(real bosons or even number of fermionic)

average

$\langle \dots \rangle = \mathrm{Tr}(\hat{\rho}\,\dots)$ with canonical $\hat{\rho}$ or grandcanonical $\hat{\rho} = \frac{1}{Z} e^{-\beta(\hat{H}-\mu\hat{N})}$

physical picture



- advanced GF (for completeness)

$$G_A(t,t') = +\frac{i}{\hbar} \langle [\hat{A}(t), \hat{B}(t')]_\varepsilon \rangle \vartheta(t'-t)$$

- causal GF (useful for T=0 diagrammatic expansion)

$$G(t,t') = -\frac{i}{\hbar} \langle T\{\hat{A}(t)\hat{B}(t')\}\rangle$$

time-ordering operator $T\{\hat{A}(t)\hat{B}(t')\} = \underbrace{\hat{A}(t)\hat{B}(t')}_{\text{normal order}}\vartheta(t-t') - \varepsilon \underbrace{\hat{B}(t')\hat{A}(t)}_{\text{reversed order}}\vartheta(t'-t)$

- thermal GF (useful for T>0 diagrammatic expansion)

uses imaginary time $\tau = it$ to unify $e^{-\frac{i}{\hbar}\hat{H}t}$ and $e^{-\beta\hat{H}}$

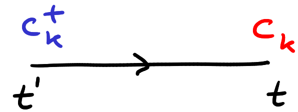
$$G(\tau,\tau') = -\frac{1}{\hbar}\langle T\{\hat{A}(-i\tau)\hat{B}(-i\tau')\}\rangle \quad \text{with} \quad \hat{A}(-i\tau) = e^{\frac{\tau}{\hbar}\hat{H}t}\hat{A}\, e^{-\frac{\tau}{\hbar}\hat{H}t}$$

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

- important examples

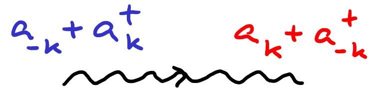
electron propagator

$$G_R(k,t) = -\frac{i}{\hbar}\langle\{c_k(t), c_k^+(t')\}\rangle\,\vartheta(t-t')$$



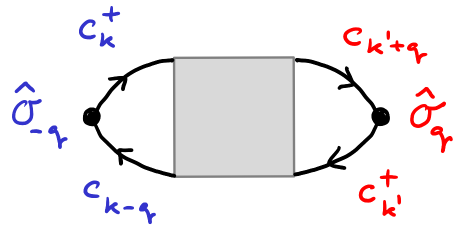
phonon propagator

$$D_R(k,t) = -\frac{i}{\hbar}\langle[\underbrace{a_k(t)+a_{-k}^+(t)}_{u_k}, \underbrace{a_{-k}(t')+a_k^+(t')}_{u_{-k}}]\rangle\,\vartheta(t-t')$$



susceptibilities (two-particle propagators)

$$\chi(q,t) = \frac{i}{\hbar}\langle[\hat{\sigma}_q(t), \hat{\sigma}_{-q}(t')]\rangle\,\vartheta(t-t')$$



$$\hat{\sigma}_q = \sum_{k\sigma\sigma'} M_{kq\sigma\sigma'}\,\hat{c}_{k\sigma}^+\,\hat{c}_{k+q\,\sigma'}$$

optical conductivity $\quad \hat{\sigma}_q = \hat{j}_q \quad (q\to 0) \quad M \sim \nabla\varepsilon_k$

spin susceptibility $\quad \hat{\sigma}_q = \hat{S}_q^z \quad M \sim \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$

• homogeneity in time (requires equilibrium and stationary $\hat{H}$)

cyclic prop. of Tr

$$\langle \hat{A}(t)\hat{B}(t')\rangle = \frac{1}{Z}\mathrm{Tr}\left(e^{-\beta\hat{H}} e^{\frac{i}{\hbar}\hat{H}t}\hat{A}\, e^{-\frac{i}{\hbar}\hat{H}t} e^{\frac{i}{\hbar}\hat{H}t'}\hat{B}\, e^{-\frac{i}{\hbar}\hat{H}t'}\right)$$

functions of $\hat{H}$ commute

$$= \frac{1}{Z}\mathrm{Tr}\left(e^{-\beta\hat{H}} e^{\frac{i}{\hbar}\hat{H}(t-t')}\hat{A}\, e^{-\frac{i}{\hbar}\hat{H}(t-t')}\hat{B}\right) = \langle \hat{A}(t-t')\hat{B}(0)\rangle$$

$$\langle \hat{B}(t')\hat{A}(t)\rangle = \frac{1}{Z}\mathrm{Tr}\left(e^{-\beta\hat{H}} e^{\frac{i}{\hbar}\hat{H}t'}\hat{B}\, e^{-\frac{i}{\hbar}\hat{H}t'} e^{\frac{i}{\hbar}\hat{H}t}\hat{A}\, e^{-\frac{i}{\hbar}\hat{H}t}\right)$$

$$= \frac{1}{Z}\mathrm{Tr}\left(e^{-\beta\hat{H}}\hat{B}\, e^{\frac{i}{\hbar}\hat{H}(t-t')}\hat{A}\, e^{-\frac{i}{\hbar}\hat{H}(t-t')}\right) = \langle \hat{B}(0)\hat{A}(t-t')\rangle$$

alltogether $G_R(t,t') = G_R(t-t')$

→ it is sufficient to consider $G_R(t) = -\frac{i}{\hbar}\langle[\hat{A}(t),\hat{B}]_\varepsilon\rangle\,\vartheta(t)$

3 Energy domain & spectral representations

- Fourier counterpart of $G_R(t)$

$$G_R(E) = \int_{-\infty}^{\infty} dt\, e^{\frac{i}{\hbar}Et}\, G_R(t)$$

$G_R(t)$ usually exponentially decays but we formally add a tiny extra damping to ensure convergence

extra damping $E \to E + i0^+$

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

using eigenbasis of $\hat{H}$

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

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

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

relabel $m \leftrightarrow n$

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

elementary Fourier transform

$$\int_{-\infty}^{\infty} dt\, e^{\frac{i}{\hbar}(E+i0^+ +E_m-E_n)t}\,\vartheta(t) = \frac{\hbar}{i}\frac{1}{E+i0^+ +E_m-E_n}\underbrace{\left[e^{\frac{i}{\hbar}(E+i0^+ +E_m-E_n)t}\right]_0^\infty}_{-1}$$

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

typical case $\hat{B}=\hat{A}^+$ $\rightarrow$ simplified $\langle m|\hat{A}|n\rangle\langle n|\hat{B}|m\rangle = |\langle n|\hat{A}^+|m\rangle|^2 = |\langle m|\hat{A}|n\rangle|^2$

$$G_R(E) = \frac{1}{Z}\sum_{mn} e^{-\beta E_m}\left[\frac{|\langle n|\hat{A}^+|m\rangle|^2}{E-(E_n-E_m)+i0^+} + \varepsilon\,\frac{|\langle n|\hat{A}|m\rangle|^2}{E+(E_n-E_m)+i0^+}\right]$$

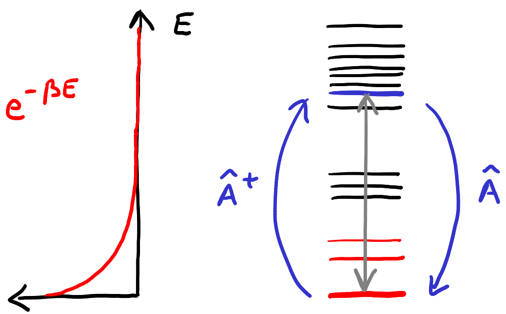
using Sochocki-Plemelj theorem $\frac{1}{x+i0^+} = \mathcal{P}\frac{1}{x} - i\pi\,\delta(x)$

spectral function $A(E) = -\frac{1}{\pi}\,\mathrm{Im}\,G_R(E) = \frac{1}{Z}\sum_{mn} e^{-\beta E_m}\,|\langle n|\hat{A}^+|m\rangle|^2\,\delta[E-(E_n-E_m)] + \dots$

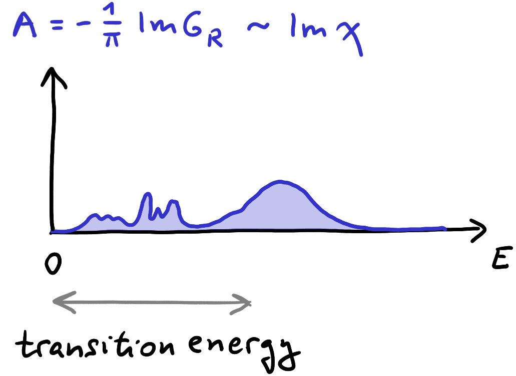
- spectral function and its interpretation ($\hat{B} = \hat{A}^+$ case)

$$A(E) = \frac{1}{Z} \sum_{mn} e^{-\beta E_m} \left\{ |\langle n|\hat{A}^+|m\rangle|^2 \delta\left[E - (E_n - E_m)\right] + \varepsilon\, |\langle n|\hat{A}|m\rangle|^2 \delta\left[E + (E_n - E_m)\right] \right\}$$

many-body energy levels



spectral function



strongly resembles Fermi golden rule

$$\frac{dP_{m\to n}}{dt} = \frac{2\pi}{\hbar} |\langle n|\hat{W}|m\rangle|^2 \left[\delta(E_n - E_m - \hbar\omega) + \delta(E_n - E_m + \hbar\omega)\right]$$

- reconstruction of $G_R(E)$

$$G(z) = \int_{-\infty}^{\infty} dE \, \frac{A(E)}{z-E} \quad \text{(Lehmann representation)} \quad \rightarrow \quad G_R(E) = G(E + i\cdot 0^+)$$

- sum rules

$$\int_{-\infty}^{\infty} dE \, A(E) = \langle [\hat{A}, \hat{A}^+]_\varepsilon \rangle \qquad \left(\text{in general } \langle [\hat{A}, \hat{B}]_\varepsilon \rangle\right)$$

$$A(E) = \frac{1}{Z} \sum_{mn} e^{-\beta E_m} \left\{ |\langle n|\hat{A}^+|m\rangle|^2 \delta[E - (E_n - E_m)] + \varepsilon |\langle n|\hat{A}|m\rangle|^2 \delta[E + (E_n - E_m)] \right\}$$

$$\hookrightarrow \int_{-\infty}^{\infty} dE \, A(E) = \frac{1}{Z} \sum_m e^{-\beta E_m} \sum_n \left(\langle m|\hat{A}|n\rangle\langle n|\hat{A}^+|m\rangle + \varepsilon \langle m|\hat{A}^+|n\rangle\langle n|\hat{A}|m\rangle \right)$$

$$\int_{-\infty}^{\infty} dE \, \frac{A(E)}{1 + \varepsilon e^{-\beta E}} = \langle \hat{A} \hat{A}^+ \rangle \qquad \left(\text{in general } \langle \hat{A} \hat{B} \rangle\right)$$

bosonic $\displaystyle\int_{-\infty}^{\infty} dE \, A(E) \, [N_B(E) + 1]$ Fermionic $\displaystyle\int_{-\infty}^{\infty} dE \, A(E) \, [1 - n_F(E)]$

- zero-temperature limit: $e^{-\beta E_m}$ picks up $|m\rangle = |GS\rangle$

$$G_R(E) = \sum_n \underbrace{\frac{|\langle n|\hat{A}^+|GS\rangle|^2}{E-(E_n-E_{GS})+i0^+}}_{\text{limited to } E>0} + \varepsilon \underbrace{\frac{|\langle n|\hat{A}|GS\rangle|^2}{E+(E_n-E_{GS})+i0^+}}_{\text{limited to } E<0}$$

connected to resolvent of $\hat{H}$ via

$$G_R(E>0) = G(E-E_{GS}+i0^+) \quad \text{with} \quad G(z) = \langle GS|\hat{A}\frac{1}{z-\hat{H}}\hat{A}^+|GS\rangle$$

T=0 spectral function

$$A(E) = \sum_n \underbrace{|\langle n|\hat{A}^+|GS\rangle|^2\,\delta[E-(E_n-E_{GS})]}_{E>0 \text{ part}} + \varepsilon \underbrace{|\langle n|\hat{A}|GS\rangle|^2\,\delta[E+(E_n-E_{GS})]}_{E<0 \text{ part}}$$