Green functions

- Notations Canonical ops c_a^+, c_a a = multi-index of before.
- $H = H_{canonical} - \mu N$ Grand canonical ensemble.
- $[H,N] = 0$ assumed.

Definition For any operator X

Thermal & quantum average

Partition function

$$\boxed{\begin{aligned} \langle X \rangle &= \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta H} X\right) \\ Z &= \mathrm{Tr}\left(e^{-\beta H}\right) \end{aligned}}$$

Definition Retarded Green Function (at $T \neq 0$)

$$\boxed{G^R_{ab}(t) = -i\theta(t) \left\langle \left\{ c_a(t), c_b^+(0) \right\} \right\rangle}$$

where $X(t) \equiv e^{+iHt} X e^{-iHt}$ (Heisenberg picture)

- Fourier conventions:

$$\boxed{\begin{aligned} f(t) &= \int \frac{d\omega}{2\pi} f(\omega) e^{-i\omega t} \\ f(\omega) &= \int dt\, f(t) e^{+i\omega t} \end{aligned}}$$

Spectral function

Definition

$$\boxed{A_{ab}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\, G^R_{ab}(\omega)}$$

$$\boxed{G^R_{ab}(\omega) = \int d\varepsilon\, \frac{A_{ab}(\varepsilon)}{\omega - \varepsilon + i0^+}}$$

eg in translation invariant case $\quad A_k(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\, G^R_k(\omega)$

with Fourier conventions

$$\begin{cases} f(t) = \int \frac{d\omega}{2\pi}\, f(\omega)\, e^{-i\omega t} \\ f(\omega) = \int dt\, f(t)\, e^{+i\omega t} \end{cases}$$

• Lehmann Representation. $T = 0$ $\rightarrow \boxed{\langle X \rangle = \langle GS | X | GS \rangle}$

$a = b = k$ case. Translation inv.

$$\boxed{A_k(\omega) = \sum_A |\langle GS | c_k | A \rangle|^2\, \delta(\omega - E_A) + \sum_B |\langle GS | c_k^+ | B \rangle|^2\, \delta(\omega + E_B).}$$

where A, B are manybody state ~~with~~. If $|GS\rangle$ has N_{GS} e^-

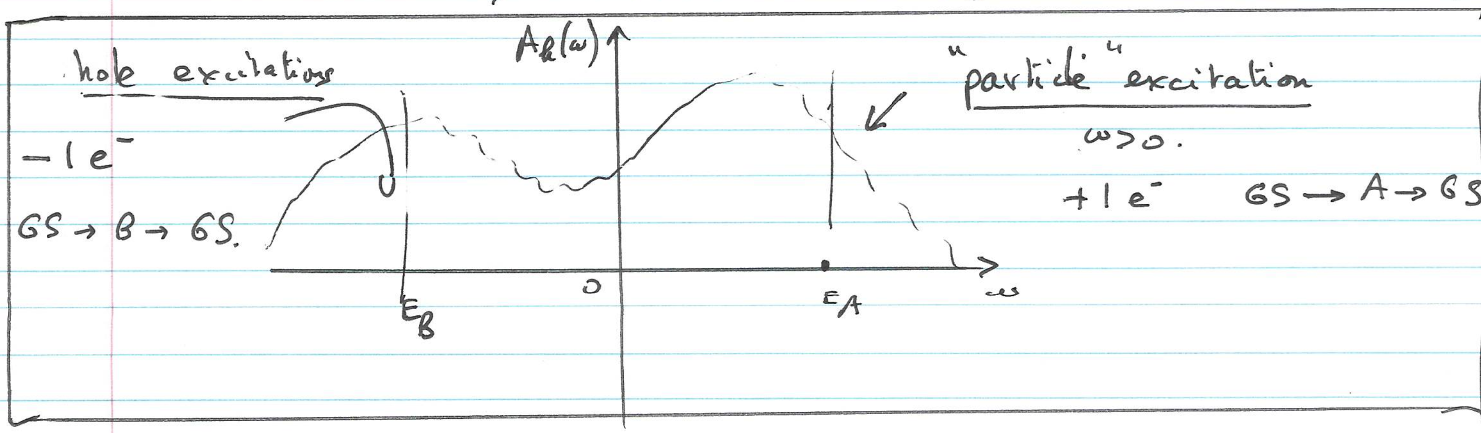
• A: $N_{GS}+1$ electrons . We assume $H|GS\rangle = 0$
  B: $N_{GS}-1$ —

Prop. $A_k(\omega) \geq 0$. $\int d\omega\, A_k(\omega) = 1$ since $\{c_k^+, c_k\} =$

. Derivation in App. 1

• Physical interpretation $A(\omega)$

• $E_A > 0$ 1) $\omega > 0$. $\omega = E_A$ only.
  $E_B > 0$.
  $A = N_{GS}+1$ electrons.
  2) $\omega < 0$ $\omega = E_B$ $N_{GS}-1$ electrons.



Lehmann representation (derivation)

$$G_k^R(t) = -i\theta(t) \langle \{ c_k(t), c_k^+(0) \} \rangle$$

$T=0 \rightarrow$
$$= -i\theta(t) \sum_A \langle GS | c_k(t) | A \rangle \langle A | c_k^+ | GS \rangle$$
$$-i\theta(t) \sum_B \langle GS | c_k^+ | B \rangle \langle B | c_k(t) | GS \rangle$$

$$c_k(t) = e^{iHt} c_k e^{-iHt}$$

$$\rightarrow G_k^R(t) = -i\theta(t) \sum_A |\langle GS | c_k | A \rangle|^2 e^{-iE_A t}$$
$$-i\theta(t) \sum_B |\langle GS | c_k^+ | B \rangle| e^{+iE_B t}$$

as
$$\left[\begin{array}{ll} H|GS\rangle = 0 & \text{by convention.} \\ H|A\rangle = E_A & \\ H|B\rangle = E_B. & \underline{\text{eigenstates}} \end{array} \right.$$

Now we use $-i\theta(t) e^{+i\alpha t} \xleftrightarrow{\text{Fourier}} \dfrac{1}{\omega+\alpha+i0^+}$

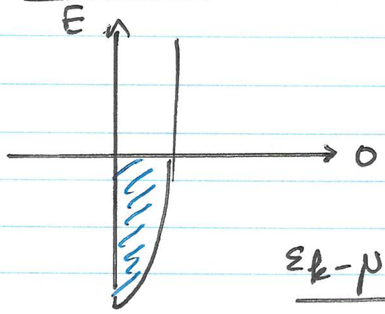
$$G_k^R(\omega) = \sum_A |\langle GS | c_k | A \rangle|^2 \frac{1}{\omega - E_A + i0^+}$$
$$+ \sum_B |\langle GS | c_k^+ | B \rangle|^2 \frac{1}{\omega + E_B + i0^+}$$

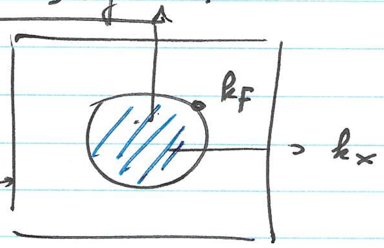
We conclude with
$$\frac{1}{\omega + i0^+} = V_p\left(\frac{1}{\omega}\right) - i\pi\delta(\omega).$$

Example 1 — Independent (free) electrons

$$H = \sum_k \varepsilon_k c_k^+ c_k - \mu N \qquad \forall \varepsilon_k$$

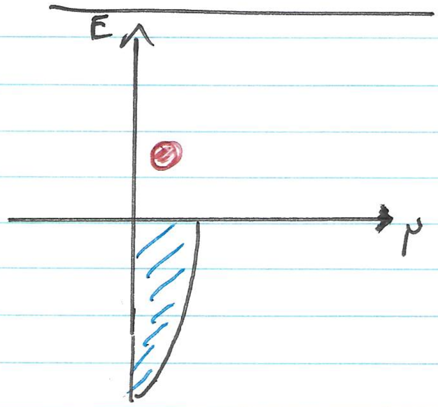
- Fermi level — Fermi Surface.



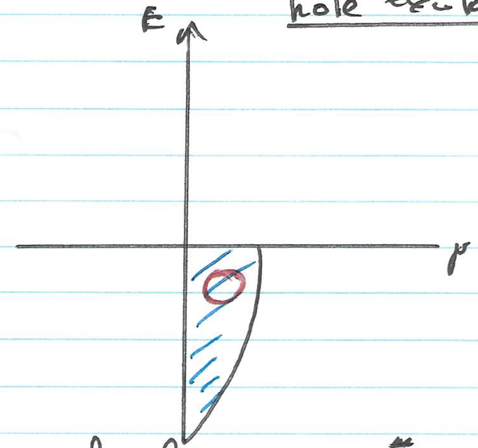


$\underline{\varepsilon_k - \mu = 0}$

- Particle excitations



hole excitation



- $k > k_F$ $\qquad E_A = \varepsilon_k - \mu > 0$
- $+1e^-$

$\omega > 0$ $\qquad \dfrac{1}{\omega - E_A} = \dfrac{1}{\omega - (\varepsilon_k - \mu)}$

$k < k_F$ $\qquad$ ~~$E_B = \varepsilon_k - \mu < 0$~~

$-1e^-$ $\qquad E_B = -(\varepsilon_k - \mu)$

$\omega < 0$ $\qquad \dfrac{1}{\omega + E_B} = \dfrac{1}{\omega + (-(\varepsilon_k - \mu))}$

$$\forall \omega \qquad \boxed{G(\omega) = \frac{1}{\omega + \mu - \varepsilon_k + i0^+}}$$

$$\boxed{A_k(\omega) = \delta(\omega + \mu - \varepsilon_k)}$$

- Other way.

$$c_k(t) = e^{iHt} c_k e^{-iHt} = e^{-i(\varepsilon_k - \mu)t} c^+$$

One more e^- here

$$G_k(t) = -i\,\theta(t) \langle [c_k(t), c_k^+\} \rangle$$
$$= -i\theta(t)\, e^{-i(\varepsilon_k - \mu)t} \xrightarrow{\text{Fourier}} \frac{1}{\omega + \mu - \varepsilon_k + i0^+}$$

Example Lehmann n°2

Hubbard atom

$$H = \varepsilon_d (n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow \quad \cancel{(-\mu N)}$$ absorbed in ε_d

4 states / Energies

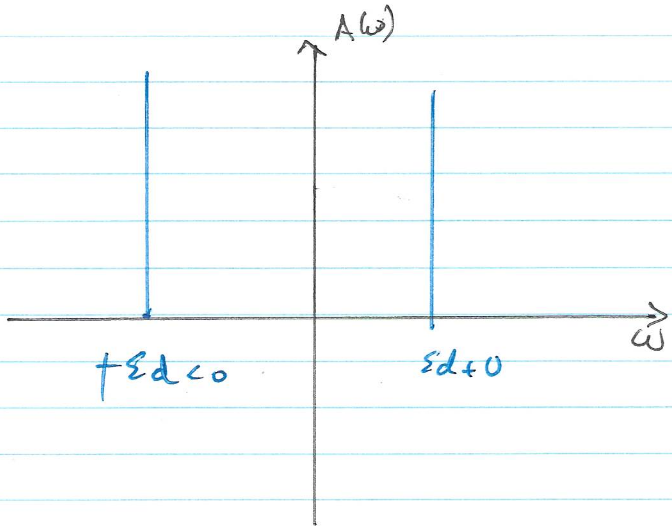
	E
$\|0\rangle$	0
$\|\uparrow\rangle, \|\downarrow\rangle$	ε_d
$\|\uparrow\downarrow\rangle$	$2\varepsilon_d + U$

- In the regime where GS is $|\uparrow\rangle |\downarrow\rangle$ i.e. $\varepsilon_d < 0$, $2\varepsilon_d + U > 0$

A : $|\uparrow\downarrow\rangle$ $\quad E_A - E_{GS} = 2\varepsilon_d + U - \varepsilon_d = \varepsilon_d + U > 0$

B $\quad |0\rangle$ $\quad E_B - E_{GS} = 0 - \varepsilon_d = -\varepsilon_d > 0$.

$$A(\omega) = \frac{1}{2}\left(\delta(\omega - \varepsilon_d) + \delta(\omega - 2\varepsilon_d - U)\right)$$

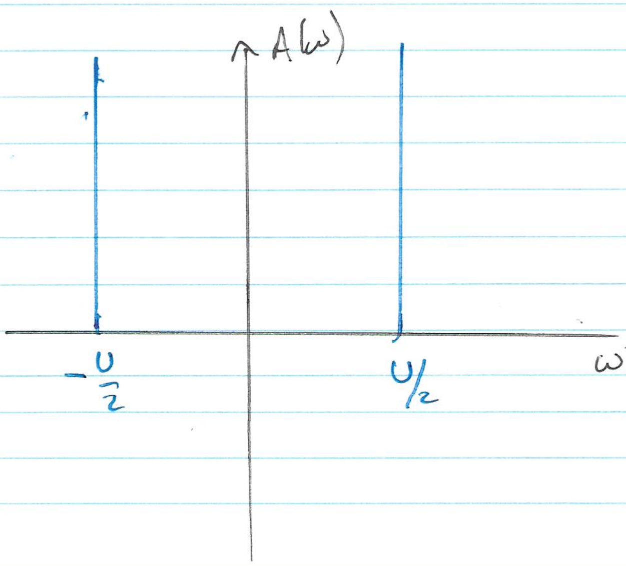


- Particle hole symmetric case

$$\varepsilon_d = -\frac{U}{2}$$

$$H = U\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right)$$

$$\boxed{A(\omega) = \frac{1}{2}\left[\delta\left(\omega - \frac{U}{2}\right) + \delta\left(\omega + \frac{U}{2}\right)\right]}$$



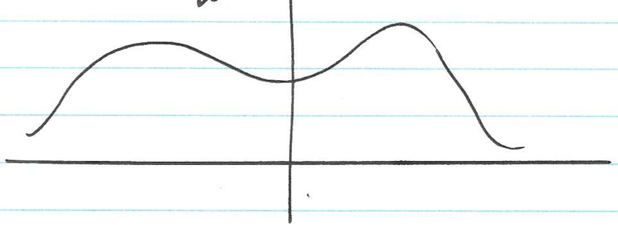
- Local Green function

$$G^R_{loc}(t) = -i\,\theta(t)\left\langle \left\{ c_{R=0}(t),\ c^\dagger_{R=0}(0) \right\} \right\rangle$$

$$\boxed{G^R_{loc}(\omega) = \sum_k G^+_k(\omega)}$$

- NB $\sum_k 1 = 1$ all Brillouin sums are normalized in these notes.

$A(\omega) = \sum_k A_k(\omega)$.



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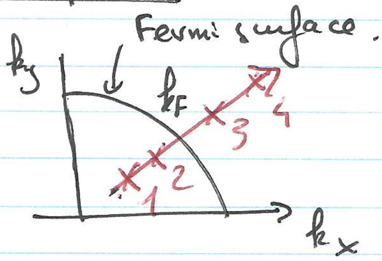
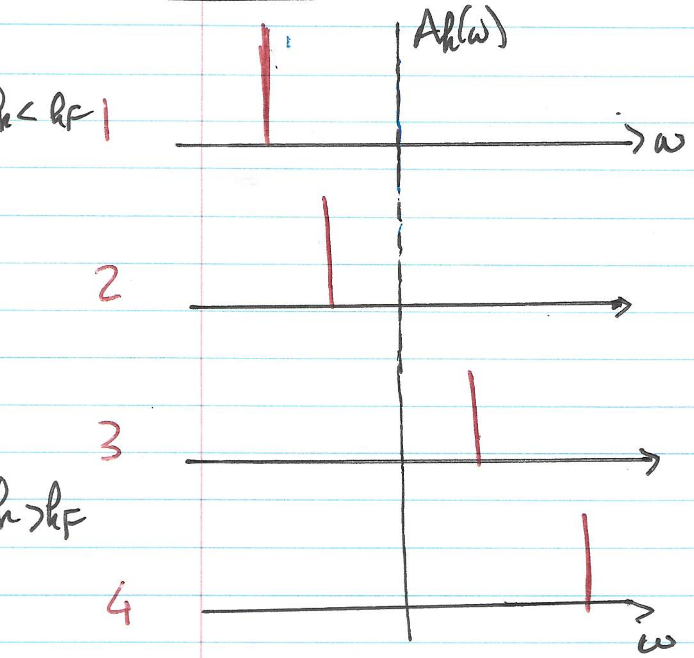
Quasi particle peak

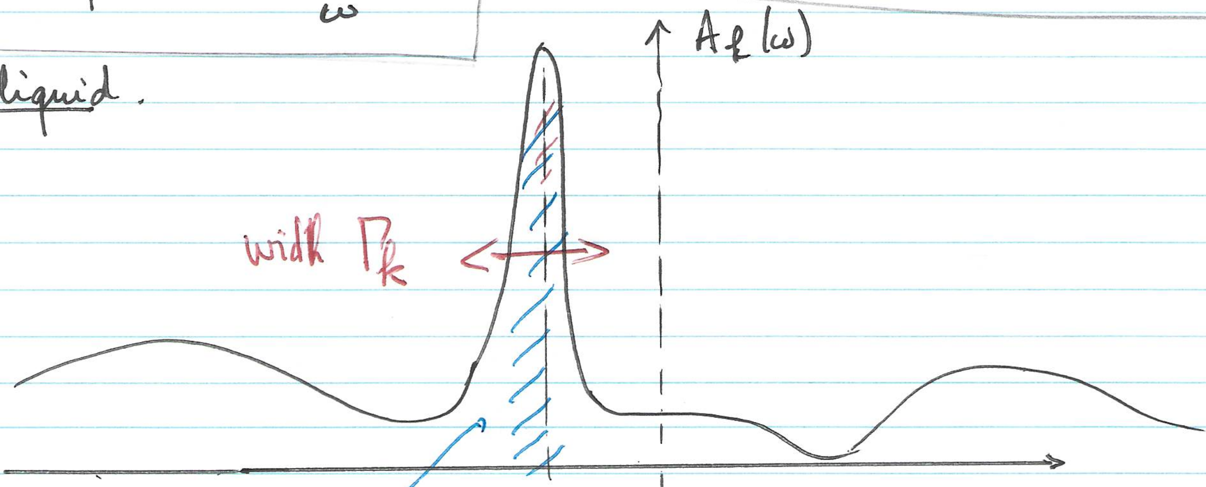
- No interaction





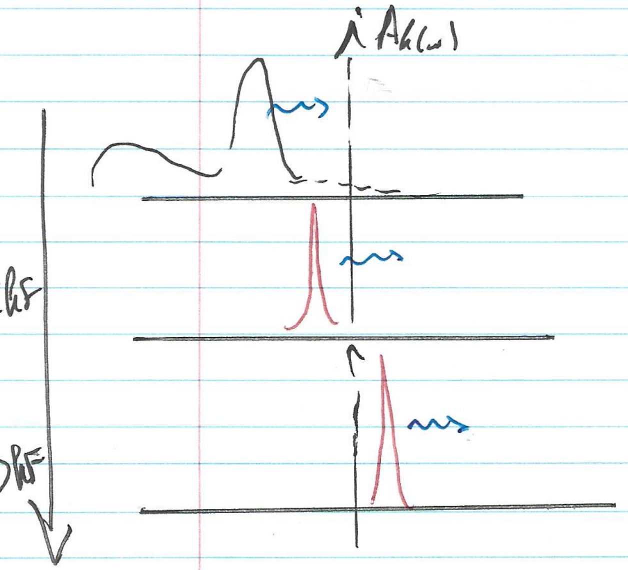
1 peak (δ) crossing Fermi surface at $k = k_F$

- Fermi liquid.



area
Z_k = quasi particle residue.

$\bar{\varepsilon}_k$ = position. ($\neq \varepsilon_k$).



- peak gets narrower close to Fermi surface.

$$\boxed{\Gamma_k \sim (\bar{\varepsilon}_k - \mu)^2}$$

(Landau 50')

Self energy

Definition

$$\boxed{G^R(\omega)^{-1} = G_0^R(\omega)^{-1} - \Sigma^R(\omega)}$$

G_0 = non-interacting (bare) Green function.

- In general, G is matrix.
- Translation invariant system:

$$G_k^{-1}(\omega) = G_{0k}^{-1}(\omega) - \Sigma_k^R(\omega)$$

$$\boxed{G_k(\omega) = \frac{1}{\omega + \mu - \varepsilon_k - \Sigma_k^R(\omega)}}$$

- Σ_k encodes the properties of quasi-particles (in a metal)
- Generalisation of Γ_k ~ frequency dependence.

Self energy in a Fermi liquid
Quasi-particle properties

- We consider low ω, T
  - $\omega, T \ll E_{coh}$ discussed later ...
- Fermi surface.

$$\underline{\mu - \varepsilon_k - \mathrm{Re}\,\Sigma^R_k(\omega=0) = 0}$$

- NB
  - Deformed by interactions $\mathrm{Re}\Sigma$ renormalises ε_k.
  - But its volume is independent of the interactions [Luttinger Theorem]

- We expand Σ at low ω, T, for $k \sim k_F$

$$\Sigma^R_k(\omega) = \mathrm{Re}\,\Sigma^R_{k_F}(0) + \left(1 - \frac{1}{Z_k}\right)\omega + (k^\perp - k_F^\perp)\,\partial_{k^\perp}\mathrm{Re}\,\Sigma^R_{k_F}(0) + i\,\mathrm{Im}\,\Sigma_{k_F}(\omega)$$

$$\mathrm{Im}\,\Sigma_k(\omega) \propto \left[\omega^2 + (\pi T)^2\right]$$

- Besides $\varepsilon_k \sim \varepsilon_{k_F} + \dfrac{(k^\perp - k_F^\perp)}{m_{band}} + \ldots$
  - m_{band} = Effective mass of electrons (due to bands)
  - $k^\perp$: expansion in orthogonal direction to Fermi Surface. (we neglect this here, take a circular shape Fermi Surface).

We have

$$G^R_k(\omega)^{-1} = \omega + \overbrace{\left[\mu - \varepsilon_{k_F} - \mathrm{Re}\,\Sigma_k\right]}^{=0} - (k-k_F)\left(\frac{1}{m_b} + \partial_k \Sigma\right) - \omega\,\partial_\omega \Sigma_k(\omega) - i\,\mathrm{Im}\,\Sigma_k(\omega)$$

$$\boxed{\begin{aligned} &\bullet\ Z_k \equiv \frac{1}{1-\partial_\omega \Sigma_k}\Big|_{\omega=0} \\ &\bullet\ \frac{m_b}{m^*} = Z_k\left(1 + m_b\,\partial_k \Sigma^R_{k_F}(\omega=0)\right) \end{aligned}}$$

$$G^R_k(\omega) = \frac{Z_k}{\omega - \frac{k-k_F}{m^*} - i\,Z_k\,\mathrm{Im}\,\Sigma_k(\omega)}$$

$\omega \sim k-k_F$

$$\boxed{\Gamma_k = Z_k\,\mathrm{Im}\,\Sigma_k(\omega \sim k-k_F)} \quad \propto (k-k_F)^2$$

$$\boxed{G^R_k(\omega) \sim \frac{Z_k}{\omega - \frac{k-k_F}{m^*} - i\,\Gamma_k}}$$

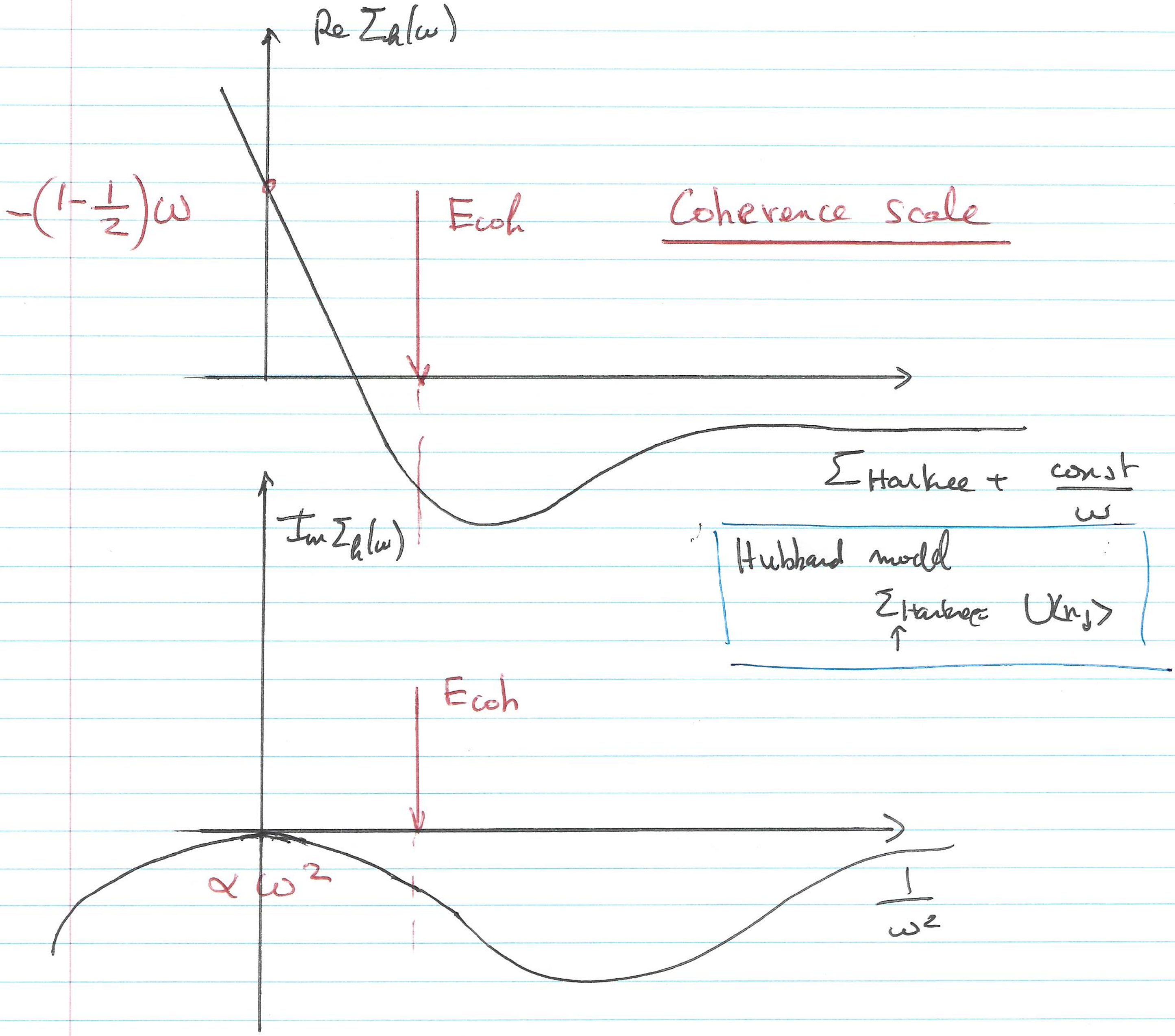
quasi particle peak (= area)

Effective mass.

width
quasi particle lifetime

· Show pic of qp peak again

Fermi liquid is a low energy theory



- $\boxed{\omega, T \ll E_{coh}}$
- Varies – E_{coh} can even vanish at some quantum phase transition.

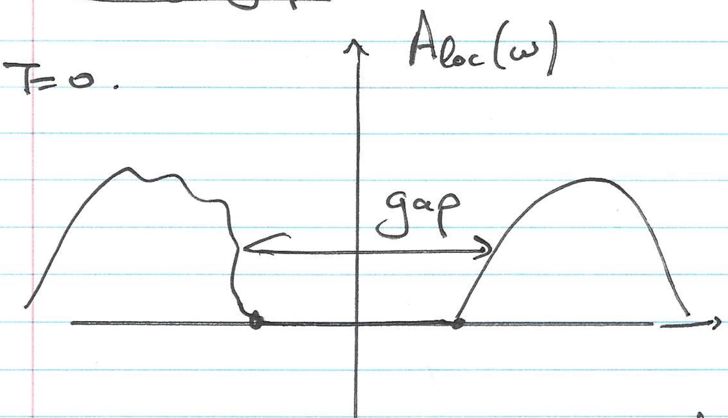
- Self energy in an insulator ?

- Well defined, but no Z_k, Γ_k .....

notions meaningless in a insulator

- charge gap

$T=0$.



- Example Hubbard atom a ~~toy~~ toy model.

$$H = \left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right).$$

$$G^R(\omega) = \frac{1}{2}\left[\frac{1}{\omega - \frac{U}{2}} + \frac{1}{\omega + \frac{U}{2}}\right]$$

$$= \frac{\omega}{\omega^2 - U^2/4} = \frac{1}{\omega - \frac{U^2}{4\omega}}$$

In this case

$$\Sigma^R(\omega) = \frac{U^2}{4\omega} \quad \text{diverges at } \omega \to 0.$$

[⚠ not always true (away from particle hole symmetry)
Σ will have poles, not necessarly at 0.]

Matsubara Green function

- Imaginary time τ $\quad 0 \leq \tau \leq \beta$. $\quad \beta = \frac{1}{T}$ $\quad (k_B = 1)$

⚠ $\tau \in \mathbb{R}$, the time evolution is imaginary

for any operator $\mathcal{O}$ $\quad \underline{\mathcal{O}(\tau) \equiv e^{H\tau}\, \mathcal{O}\, e^{-H\tau}}$ $\quad [\tau = it]$

we assume $E_{GS} = 0$ $\quad H \geq 0$.

- <u>Definition</u>

$$\boxed{G_{ab}(\tau - \tau') = -\langle T_\tau\, c_a(\tau)\, c_b^+(\tau') \rangle}$$

w/ T_τ: time ordering operator.

$$T_\tau A(\tau) B(\tau') = \theta(\tau - \tau')\, A(\tau)\, B(\tau') + \zeta_{AB}\, \theta(\tau' - \tau)\, B(\tau')\, A(\tau)$$

with $\zeta_{AB} = \begin{cases} -1 & \text{if both } A, B \text{ are fermionic} \\ 1 & \text{else} \end{cases}$

- NB: Under T_τ operators (anti-) commute.

- $G(\tau)$ is defined on $-\beta \leq \tau - \tau' \lesseqgtr \beta$.

  We define it to be 2β - periodic on $\mathbb{R}$.

- <u>Fermions</u>: $\quad G_{ab}(\tau + \beta) = -G_{ab}(\tau) \quad$ for $-\beta \leq \tau \leq 0$

  (bosons) $\quad G_{ab}(\tau + \beta) = +G_{ab}(\tau) \quad$ —

$\rightarrow$ <u>$G_{ab}(\tau)$ is β-(anti-) periodic</u> $\quad$ Proof of App.

⚠ . [<u>Motivation</u> – Solvers, QMC, methods works in Matsubara

Matsubara frequencies

$$\boxed{\begin{aligned} \omega_n &= \frac{(2n+1)\pi}{\beta} && \text{Fermions} \\ \nu_n &= \frac{2n\pi}{\beta} && \text{Bosons} \end{aligned}}$$

$$\boxed{\begin{aligned} G_{ab}(\tau) &= \frac{1}{\beta} \sum_{n \in \mathbb{Z}}{}' \; e^{-i\omega_n \tau} \; G_{ab}(i\omega_n) \\ G_{ab}(i\omega_n) &= \int_0^\beta d\tau \; G(\tau) \, e^{i\omega_n \tau} \end{aligned}}$$

Proof 1. $\boxed{G_{ab}(\tau+\beta) = -G_{ab}(\tau)}$ $\quad -\beta \leq \tau \leq 0$.

$$\mathrm{Tr}\left(e^{-\beta H} \cancel{T}\; e^{H(\tau+\beta)} c_a\, e^{-H(\tau+\beta)}\, c_b^{+}\right)$$

$\tau+\beta > 0$, remove T $\quad$ ~~$\tau+\beta$~~

$$= \mathrm{Tr}\left(e^{H\tau} c_a\, e^{-\beta H} e^{-H\tau} c_b^{+}\right)$$

$$= \mathrm{Tr}\left(e^{-\beta H} c_b^{+}\, e^{H\tau} c_a\, e^{-H\tau}\right)$$

$$= \mathrm{Tr}\left(e^{-\beta H} c_b^{+}\, c_a(\tau)\right) \quad \text{but } \tau < 0$$

$$= -\mathrm{Tr}\left(e^{-\beta H}\, T\, c_a(\tau)\, c_b^{+}\right) = -G_{ab}(\tau).$$

Spectral representation.

(I) $$G^R_{ab}(t-t') = -i\,\theta(t-t')\,\langle \{ c_a(t), c_b^+(t')\} \rangle$$

$T \neq 0$ now.

$$G^R_{ab}(\omega) = \int d\omega' \, \frac{A_{ab}(\omega')}{\omega - \omega' + i0^+}$$

Lehmann $T>0$

$$\boxed{A_{ab}(\omega) = \frac{1}{Z} \sum_{AB} \langle A | c_a | B \rangle \langle B | c_b^+ | A \rangle \left(e^{-\beta E_A} + e^{-\beta E_B} \right) \times \delta(\omega + E_A - E_B)}$$

- Generalisation to finite temperature

⚠ in interacting systems, $A(\omega)$ depends on T.

(II) $$G_{ab}(\tau) = -\langle T_\tau \, c_a(\tau) \, c_b^+ \rangle \qquad 0 \leq \tau \leq \beta.$$

$$= -\frac{1}{Z} \sum_{AB} e^{-\beta E_A} \langle A | c_a(\tau) | B \rangle \langle B | c_b^+ | A \rangle$$

$$= -\frac{1}{Z} \sum_{AB} e^{-\beta E_A} \langle A | c_a | B \rangle \langle B | c_b^+ | A \rangle \, e^{(E_A - E_B)\tau}$$

$$\int_0^\beta e^{i\omega_n \tau + (E_A - E_B)\tau} d\tau = (-) \frac{e^{\beta(E_A - E_B)} + 1}{i\omega_n + E_A - E_B}$$

$$G_{ab}(i\omega_n) = + \frac{1}{Z} \sum_{AB} \langle A | c_a | B \rangle \langle B | c_b^+ | A \rangle \frac{e^{-\beta E_A}\left(e^{\beta(E_A - E_B)} + 1\right)}{i\omega_n + E_A - E_B}.$$

$$\boxed{G_{ab}(i\omega_n) = \int d\varepsilon \, \frac{A_{ab}(\varepsilon)}{i\omega_n - \varepsilon}}$$

$$\boxed{G_{ab}(\tau) = -\int d\varepsilon \, A_{ab}(\varepsilon) \frac{e^{-\varepsilon\tau}}{1 + e^{-\beta\varepsilon}}} \qquad 0 \leq \tau \leq \beta.$$

$\boxed{\text{App.}}$ Proof finite T spectral representation

$$\begin{cases} G^{>}_{ab}(t) = -i \langle c_a(t)\, c_b^{+} \rangle \\ G^{<}_{ab}(t) = +i \langle c_b^{+}\, c_a(t) \rangle \end{cases}$$

- $$G^{>}_{ab}(t) = -\frac{i}{Z} \operatorname{Tr}\left(\underset{|A\rangle}{e^{-\beta H}}\; e^{iHt} c_a \underset{|B\rangle}{e^{-iHt}} c_b^{+} \right)$$

$$= -\frac{i}{Z} \sum_{AB} e^{-\beta E_A} e^{i(E_A - E_B)t} \langle A | c_a | B \rangle \langle B | c_b^{+} | A \rangle$$

- $$G^{<}_{ab}(t) = +\frac{i}{Z} \sum_{AB} e^{-\beta E_B} e^{i(E_A - E_B)t} \langle B | c_b^{+} | A \rangle \langle A | c_a | B \rangle$$

$$\left(\operatorname{Tr}\left(\underset{B}{e^{-\beta H}} c_b^{+}\, \underset{A}{e^{iHt}} c_a e^{-iHt} \right) \right)$$

- $$G^{R}_{ab}(t) = \Theta(t) \left(G^{>}_{ab}(t) - G^{<}_{ab}(t) \right)$$

$$-i\,\Theta(t)\, e^{i\alpha t} \to \frac{1}{\omega + \alpha + i0^{+}} \longrightarrow \delta(\omega + \alpha).$$

$$\left[\; A_{ab}(\omega) = \frac{1}{Z} \sum_{AB} \langle A | c_a | B \rangle \langle B | c_b^{+} | A \rangle\, \delta(\omega + E_A - E_B) \left(e^{-\beta E_A} + e^{-\beta E_B} \right). \right.$$

$\square$

What can we extract from Matsubara formalism?

Yes

- Static correlations

  eg $n_k = \langle c_k^\dagger c_k \rangle$, $\langle H \rangle$

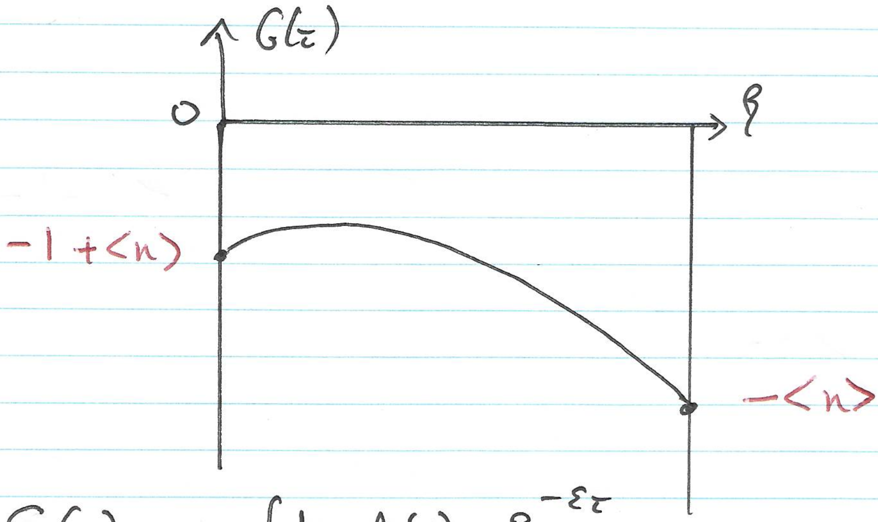
- Thermodynamics (F, C, ...)
- Low energy behaviour.

No (or hard, require analytic continuation).

- $A_k(\omega)$ (ω not small)
- Transport
- $\omega \ll T$ regime.

Sketch of $G(\tau)$

- local Green function $G(\tau)$.



$G(\tau) \leq 0$

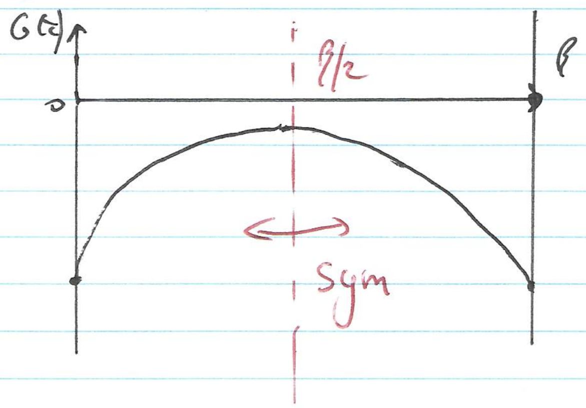
- $G(\tau) = -\int d\varepsilon \, A(\varepsilon) \, \dfrac{e^{-\varepsilon\tau}}{1+e^{-\beta\varepsilon}}$

$$\left[\begin{array}{l} G(\tau) \leq 0 \\ \partial_\tau^2 G(\tau) \leq 0 \\ \quad [\text{Concave}] \end{array}\right.$$

discontinuity $\left[\begin{array}{l} G(\tau=0^+) - G(\tau=0^-) = -1 \\ G(\tau=0^+) + G(\tau=\beta^-) = -1 \end{array}\right.$

$\left[\begin{array}{l} G(\tau=0^-) = \langle n\rangle \\ \text{Number of particles} \end{array}\right.$

- <u>Particle-hole symmetric case</u>



$G(\beta-\tau) = G(\tau)$

<u>Exercise:</u>
equivalent to $A(\omega) = A(-\omega)$

Exercise solution:

$$G(\tau) = -\int d\varepsilon \; A(\varepsilon) \frac{e^{-\varepsilon\tau}}{1+e^{-\beta\varepsilon}} \qquad 0 \leq \tau \leq \beta$$

$$G(\beta-\tau) = -\int d\varepsilon \; A(\varepsilon) \frac{e^{-\beta\varepsilon} \, e^{+\varepsilon\tau}}{1+e^{-\beta\varepsilon}}$$

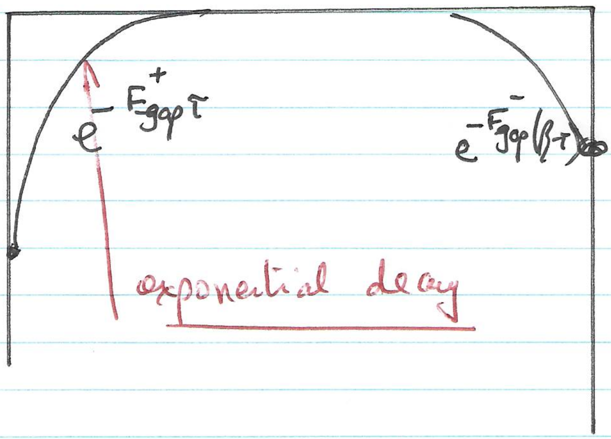
$\varepsilon \longleftrightarrow -\varepsilon$

$$= -\int d\varepsilon \; A(-\varepsilon) \; e^{-\varepsilon\tau} \frac{1}{e^{-\beta\varepsilon}+1}$$

$$\boxed{G(\beta-\tau) \longleftrightarrow A(-\varepsilon)}$$

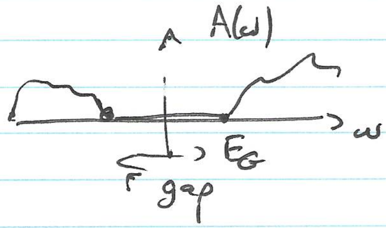
$G(\tau)$ in insulator

Insulator



- $$G(\tau) = \int d\varepsilon \, A(\varepsilon) \frac{e^{-\varepsilon\tau}}{1+e^{-\beta\varepsilon}}$$

$$G(\tau) \sim e^{-E_{gap}\tau}$$



Toy example

Hubbard atom

$$G(\tau) = \frac{1}{2}\left[\frac{e^{-\frac{U}{2}\tau}}{1+e^{-\frac{\beta U}{2}}} + \frac{e^{U\tau}}{1+e^{+\frac{\beta U}{2}}} \right]$$

Anatomy of $G(\tau)$: metal

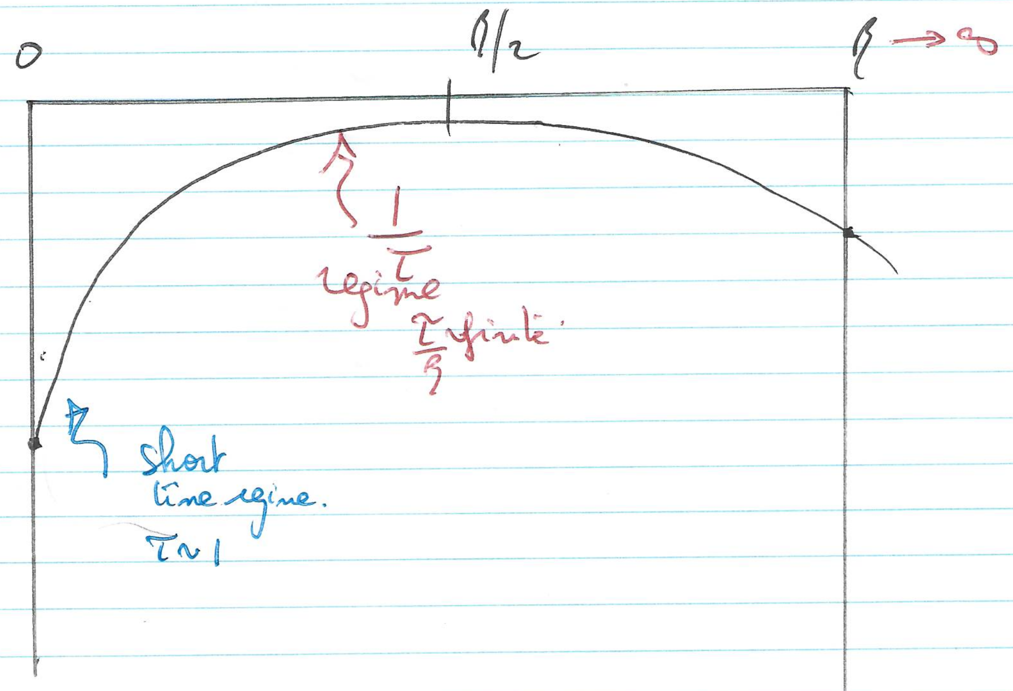
- Local $G(\tau)$ in a metal

$T=0$ $\left[\begin{array}{l} G(\tau) \sim \dfrac{1}{\tau} \\ \langle S(0) S(\tau) \rangle \sim \dfrac{1}{\tau^2} \end{array} \right.$ Fermi liquid.

long time = low energy.

- Issue
  - how to see that?
  - But $\beta < \infty$, τ is bounded ??

- We take $T \to 0$, $\beta \to \infty$ limit, τ/β fixed.



$$\boxed{G(\tau) \sim A(0) \left(\frac{\pi/\beta}{\sin \frac{\pi \tau}{\beta}} \right)}$$

$\tau, \beta \to \infty$
t/β fixed.

- $T \neq 0$

$\beta \to \infty$ $\quad \frac{\tau}{\beta} \ll 1$ regime. $\quad \boxed{G(\tau) \sim \frac{1}{\tau}}$

$D^{-1} \ll \tau \ll \beta$ $\quad \boxed{G(\beta/2) \sim A(0)}$

~~Slide~~
~~eg SYK paper~~

Proof of scaling for $G(\tau)$

$x = \beta\varepsilon$

$$G(\tau) = -\int d\varepsilon\, A(\varepsilon)\,\frac{e^{-\varepsilon\tau}}{1+e^{-\beta\varepsilon}} = -\int \frac{dx}{\beta}\, A\left(\frac{x}{\beta}\right)\frac{e^{-\cancel{x}\tau/\beta}}{1+e^{-x}}$$

$A\left(\frac{x}{\beta}\right) \sim A(0)$ $\qquad G(\tau) = -\frac{A(0)}{\beta}\int_{-\infty}^{+\infty} dx\, \frac{e^{-x(\tau/\beta)}}{1+e^{-x}}$

$y = e^{-x\frac{\tau}{\beta}}$, $\quad dy = y(-)\frac{\tau}{\beta}dx$

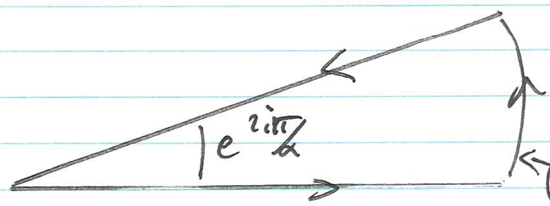
$$G(\tau) = -\frac{A(0)}{\beta}\int_0^{\infty}\frac{dy}{\left(\frac{\tau}{\beta}\right)y}\,\frac{y}{1+y^{\beta/\tau}}$$

$$G(\tau) = -\frac{A(0)}{\tau}\int_0^{\infty}\frac{dy}{1+y^{\beta/\tau}}$$

But $\quad I_\alpha = \int_0^\infty \frac{dy}{1+y^\alpha} = \frac{\pi/\alpha}{\sin \pi/\alpha} \quad$ for $\alpha > 1$

hence $\quad \boxed{G(\tau) = -\frac{A(0)}{\tau}\,\frac{\pi\,\tau/\beta}{\sin \pi\tau/\beta}}$ $\quad\square$.

- Compute I_α by contour integral $\qquad I_\alpha = \int_0^\infty \frac{dy}{1+y^\alpha}$



$\left(I_\alpha - e^{\frac{2i\pi}{\alpha}} I_\alpha\right) = 2i\pi$ Resid

$\left(\frac{R}{R^{\alpha+1}} \to 0 \quad R\to\infty \quad \text{since } \alpha > 1\right)$

1 pole at $\quad y^\alpha = -1 \qquad y = e^{\frac{i\pi}{\alpha}} \to \text{Res} = \frac{1}{\alpha y^{\alpha-1}} = -\frac{y}{\alpha} = -\frac{e^{i\pi/\alpha}}{\alpha}$

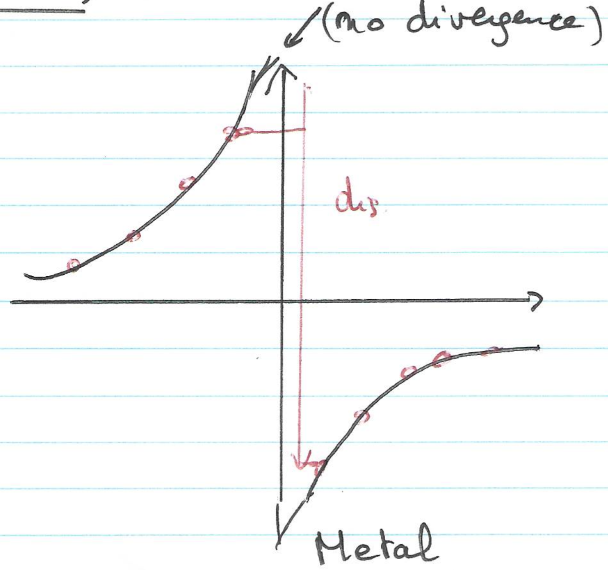
$$I_\alpha\left(1 - e^{2i\pi/\alpha}\right) = 2i\pi\,\text{Res}$$

$$-I_\alpha\,(2i)\sin \pi/\alpha\; e^{i\pi/\alpha} = 2i\pi(-1)\frac{e^{i\pi/\alpha}}{\alpha}$$

$$\boxed{I_\alpha = \frac{\pi/\alpha}{\sin \pi/\alpha}}$$

Sketch of $G(i\omega_n)$

Insulator



Metal

- Analyze $\omega_n \to 0^+, 0^-$ discontinuity
- at $\beta \to \infty$, value at $G(i\omega_n)$ accumulate / slide on a (black) curve
- $$G(z = i0^+) - G(z = -i0^+)$$
  $$= -\int d\varepsilon\, A(\varepsilon) \underbrace{\left[\frac{1}{\varepsilon - i0^+} - \frac{1}{\varepsilon + i0^+}\right]}_{\propto\, \delta(\varepsilon)} \propto A(0)$$

"Discontinuity" $G(\omega_n \to 0^+) - G(\omega_n \to 0^-) \propto A(0)$.

Anatomy of a metallic selfenergy

$\Sigma(i\omega_n)$

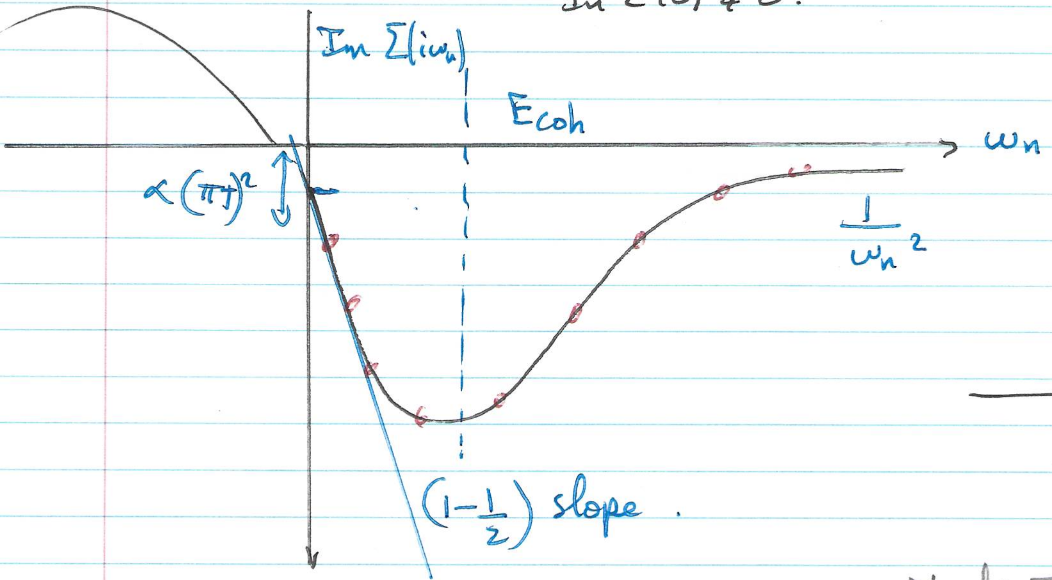
Reminder (local selfenergy)

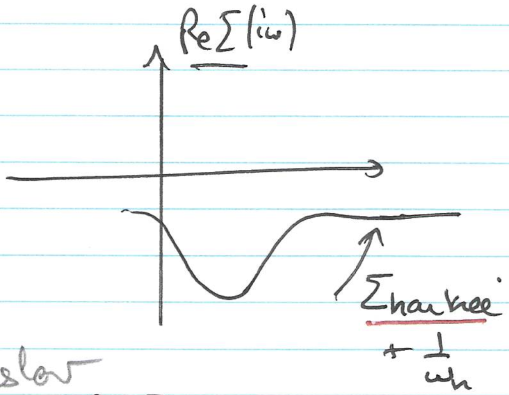
$$\Sigma^R(\omega) = \mathrm{Re}\,\Sigma^R(0) + \left(1-\frac{1}{Z}\right)\omega + ic\left(\omega^2+(\pi T)^2\right)$$

In Matsubara:

$$\Sigma(i\omega_n) = \mathrm{Re}\,\Sigma(\omega_n\to 0) + \left(1-\frac{1}{Z}\right) i\omega_n + ic\left((\pi T)^2-\omega_n^2\right) + \dots$$

- Z is now part of $\mathrm{Im}\,\Sigma(i\omega_n)$ instead of $\mathrm{Re}\,\Sigma^R(\omega)$.
- A finite T, $\mathrm{Re}\,\Sigma(0) \neq 0$. $\mathrm{Im}\,\Sigma(0) \neq 0$.





- Fermi liquid 1st at low energy [Maslov Chubukov]

$$\Sigma_1(i\omega_0) = \text{const} + \left(1-\frac{1}{Z}\right) i\omega_0 + ic\left(\underbrace{(\pi T)^2-\omega_0^2}_{=0}\right) + O\dots$$

$\omega_0 = \pi T$

$$\boxed{\Sigma(i\pi T) = \text{conste} + \left(1-\frac{1}{Z}\right) i\pi T + O(T^3)}$$

- Linear behavior at low T.

slide show example.

Σ in an insulator

- Toy model : Hubbard atom

$$G = \frac{1}{2}\left[\frac{1}{i\omega_n - \frac{U}{2}} + \frac{1}{i\omega_n + \frac{U}{2}}\right]$$

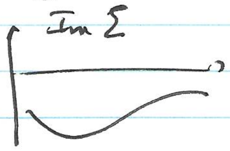
$$\Sigma = \frac{U^2}{4 i\omega_n} \xrightarrow[\omega_n \to 0]{} \infty$$

Non Fermi liquid clearly...

⚠ Σ : Insulator $\not\Longrightarrow$ $\Sigma(\omega_n) \xrightarrow[\omega_n \to 0]{} \infty$

depends on position of pole of Σ

- Σ can look deceivingly simple



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Methodology

1. Look at $G(\tau)$, $G(i\omega_n)$

2. In metal, analyse Σ.

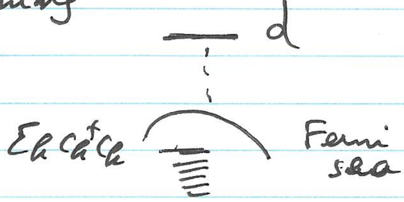
Non interacting impurity model

• Hamiltonian : 1 level d coupled to a bath of non interacting fermion

$$H = \varepsilon_d d^\dagger d + \sum_{\lambda=1}^{N_\lambda} \varepsilon_\lambda c_\lambda^\dagger c_\lambda + \sum_{\lambda=1}^{N_\lambda} V_\lambda d^\dagger c_\lambda + V_\lambda^* c_\lambda^\dagger d$$

nb : - no spin . Calculation is independent of spin.

- λ can be anything
  - $\lambda = k$



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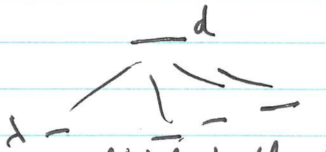


multiple bath site
no translation invariance.

• Order the operators: $\xi = \begin{pmatrix} c_\lambda \\ \vdots \\ d \end{pmatrix}$

Then: $H = \xi^\dagger M \xi$ with $M = \left[\begin{array}{cc|c} \varepsilon_\lambda & 0 & \\ 0 & \varepsilon_\lambda & V_\lambda^* \\ \hline & V_\lambda & \varepsilon_d \end{array}\right]$

Hence: $G(i\omega_n)^{-1} = \left[\begin{array}{cc|c} i\omega_n - \varepsilon_\lambda & & -V_\lambda^* \\ & i\omega_n - \varepsilon_\lambda & \\ \hline & -V_\lambda & i\omega_n - \varepsilon_d \end{array}\right]$

Define $G = \begin{array}{c} \left[\begin{array}{c|c} G_{cc} & G_{cd} \\ \hline G_{dc} & G_{dd} \end{array}\right] \begin{array}{l} \updownarrow N_\lambda \\ \updownarrow 1 \end{array} \\ \overset{\longleftrightarrow}{N_\lambda} \quad \overset{\longleftrightarrow}{1} \end{array}$

Using Schur complement formula: (cf Next page)

$$G_{dd}(z) = z - \varepsilon_d - \sum_\lambda V_\lambda \frac{1}{\cancel{i\omega_n} z - \varepsilon_\lambda} V_\lambda^*$$

$$\boxed{G_{dd}(z) = \frac{1}{z - \varepsilon_d - \sum_\lambda \frac{|V_\lambda|^2}{z - \varepsilon_\lambda}}}$$

Schur complement

- We have a matrix by block

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \qquad A_{11} \text{ invertible}$$

- Schur complement is defined by

$$\boxed{[A/A_{11}] \equiv A_{22} - A_{21}(A_{11})^{-1}A_{12}} \qquad \text{sector } 2\times 2$$

Then

① $$\boxed{[A^{-1}]_{22} = [A/A_{11}]^{-1}}$$

② $$\boxed{\det A = \det A_{11} \det [A/A_{11}]}$$

- Proof $$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ A_{21}A_{11}^{-1} & 1 \end{pmatrix} \begin{pmatrix} A_{11} & 0 \\ 0 & [A/A_{11}] \end{pmatrix} \begin{pmatrix} 1 & A_{11}^{-1}A_{12} \\ 0 & 1 \end{pmatrix}$$

by direct inspection (do the product).

② is then obvious.

- A block matrix of the form

$$\begin{pmatrix} 1 & 0 \\ X & 1 \end{pmatrix} \text{ is easy to invert as } \begin{pmatrix} 1 & 0 \\ X & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ -X & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$A^{-1} = \begin{pmatrix} 1 & -A_{11}^{-1}A_{12} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} A_{11}^{-1} & 0 \\ 0 & [A/A_{11}]^{-1} \end{pmatrix} \begin{pmatrix} 1 & \cancel{A_{11}^{-1}A_{12}}\ 0 \\ -A_{21}A_{11}^{-1} & 1 \end{pmatrix}$$

hence $[A^{-1}]_{22} = [A/A_{11}]^{-1}$ which ①.

Hybridization function

Definition:

$$\boxed{\begin{aligned} \Delta(i\omega_n) &\equiv \sum_\lambda \frac{|V_\lambda|^2}{i\omega_n - \varepsilon_\lambda} \\ G_{dd}(i\omega_n)^{-1} &= i\omega_n - \varepsilon_d - \Delta(i\omega_n) \end{aligned}}$$

- From now on, $G_d \equiv G_{dd}$.
- <u>NB</u> Details of the bath only enter through Δ

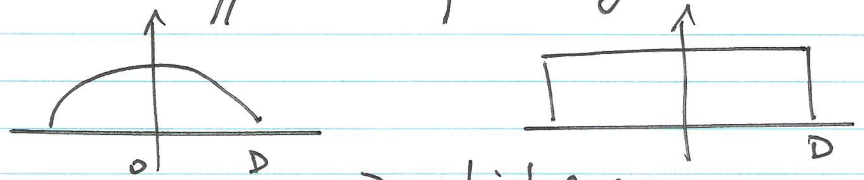
Hybridization function
Continuous limit

- when $N_d < \infty$, Δ is a set of δ - peaks
- Continuous limit, eg $d =$ Fermi sea

$$\Delta^R(\omega) = \sum_k \frac{|V_k|^2}{\omega - \varepsilon_k + i0^+} \qquad \Delta''(\omega) \equiv -\frac{1}{\pi} \operatorname{Im} \Delta^R(\omega).$$

$$\Delta''(\omega) = \sum_k |V_k|^2 \delta(\omega - \varepsilon_k)$$

- Δ'' can have different shapes eg



flat band (useful for theorists)

$D =$ high energy cut off $\sim eV$

- Assuming: low energy $|\omega|, |\varepsilon_d| \ll D$ and $|V_k|$ independant of k (not crucial)

we get $\Delta^R(\omega \sim 0) = \operatorname{Re} \Delta^R(0) - i\pi |V|^2 \rho_0(0)$

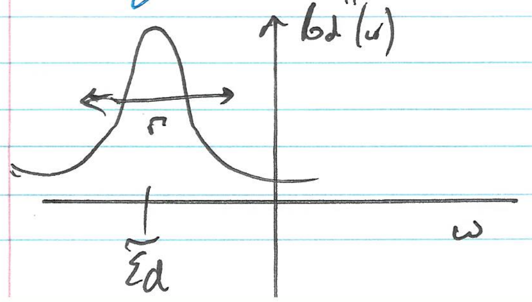
with $\rho_0(\omega) = \sum_k \delta(\omega - \varepsilon_k)$ d.o.s of the electronic bath.

$\tilde{\varepsilon}_d = \varepsilon_d + \operatorname{Re} \Delta^R(0)$.

$$\boxed{G_d^R(\omega) \simeq \frac{1}{\omega - \tilde{\varepsilon}_d + i\Gamma} \qquad \Gamma = \pi |V|^2 \rho_0(0)}$$

d.o.s at Fermi level

Lorentzian



Fermi Golden rule

- 1 level coupled to a continuum of states

Action form

$$H = \varepsilon_d d^+ d + \sum_\lambda \varepsilon_\lambda c_\lambda^+ c_\lambda + \sum_\lambda V_\lambda d^+ c_\lambda + V_\lambda^* c_\lambda^+ d$$

$$Z = \int \mathcal{D}c\,\mathcal{D}d \ \exp\left(-S(c,d)\right)$$ Grassman path integral (fermions)

$$S = \int d\tau \ d^+(\tau)\left(-\partial_\tau - \varepsilon_d\right) d(\tau) + \underbrace{V^* c_\lambda^+ d + h.c}_{\text{source for } c_\lambda^+}$$
$$\bar{c}_\lambda(\tau)\left(-\partial_\tau - \varepsilon_\lambda\right) c_\lambda(\tau) \ \ldots$$

Or in frequencies $\quad S = \sum_n{}' \ \bar{c}_{\lambda i\omega_n}\left(i\omega_n - \varepsilon_d\right) c_{\lambda i\omega_n} + \ldots$

- Quadratic. Gaussian integral

<u>Integrate the bath</u> $\quad Z = \int \mathcal{D}d \ e^{-S_{eff}(\bar{d},d)}$

by integrating the $\underline{c_\lambda}$.

$$S = \sum_\lambda \left(i\omega_n - \varepsilon_\lambda\right)\underbrace{\left(\bar{c}_\lambda + \frac{V_\lambda^* \bar{d}}{i\omega_n - \varepsilon_\lambda}\right)}_{\bar{\tilde{c}}}\underbrace{\left(c_\lambda + \frac{V_\lambda d}{i\omega_n - \varepsilon_\lambda}\right)}_{\tilde{c}} - \underbrace{\sum_\lambda \frac{V_\lambda^* V_\lambda}{i\omega_n - \varepsilon_\lambda}}_{\Delta(i\omega_n)} \bar{d}_{i\omega_n} d_{i\omega_n}$$

$$Z = \int \mathcal{D}\tilde{c}\,\mathcal{D}d \ e^{-(\ldots \bar{\tilde{c}}\,\tilde{c}) + \ldots \bar{d}\,d}$$ change variable.

$$c \to \tilde{c}_\lambda = \frac{V_\lambda d}{i\omega_n - \varepsilon_\lambda} + c_\lambda$$

$$S_{eff} = \bar{d}\left(i\omega_n - \varepsilon_d - \Delta(i\omega_n)\right) d$$

$$\boxed{\begin{aligned} \mathcal{G}_0^{-1} &= i\omega_n - \varepsilon_d - \Delta(i\omega_n) \\ S_{eff} &= -\int d\tau d\tau' \ d^+(\tau)\ \mathcal{G}_0^{-1}(\tau-\tau')\ d(\tau') \end{aligned}}$$

Quadratic effective action for $\underline{d}$

- bath $\to$ all details go to $\Delta(i\omega_n)$.

Anderson model

$$\boxed{H = \varepsilon_d d_\sigma^+ d_\sigma + \sum_\lambda \varepsilon_\lambda c_{\lambda\sigma}^+ c_{\lambda\sigma} + \sum_\lambda V_\lambda d_\sigma^+ c_{\lambda\sigma} + h.c. + U n_{d\uparrow} n_{d\downarrow}.}$$

- Spin $\sigma = \uparrow, \downarrow$. Crucial
- $\underline{U=0}$ 2 copies of previous non interacting model
- $V_\lambda = 0$ $(\Delta = 0)$: Hubbard atom. (cf before).

- Action form

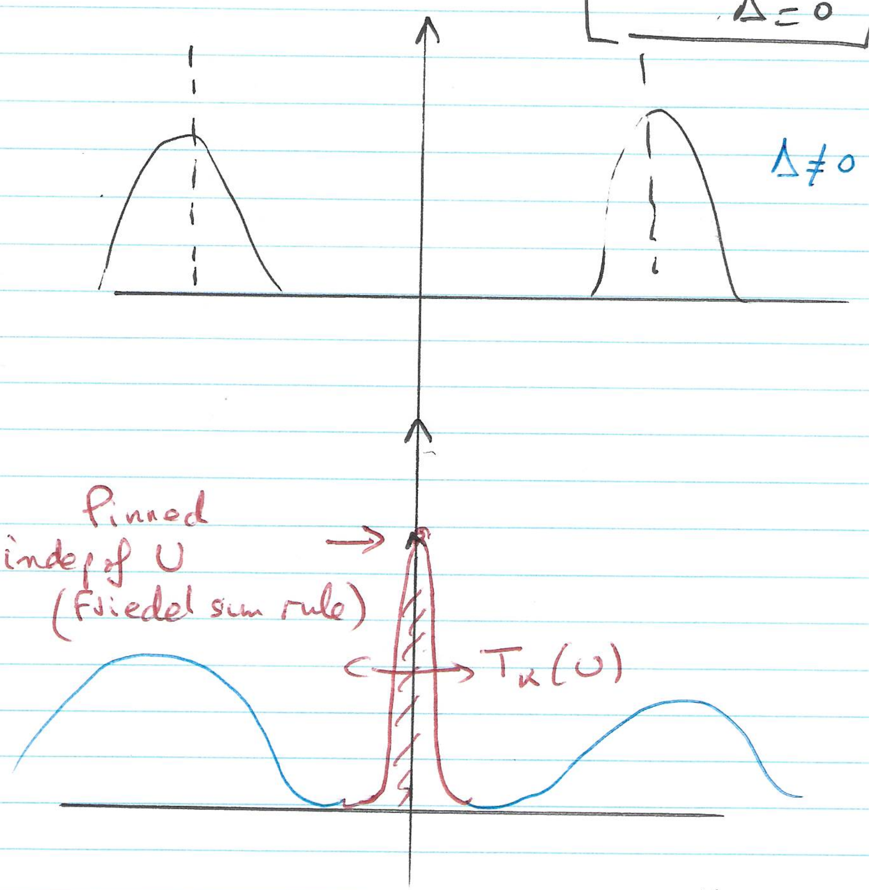
  - $U n_{d\uparrow} n_{d\downarrow}$ does not participate to integration.

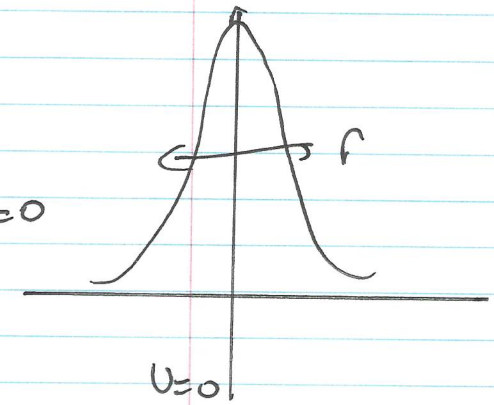
$$\boxed{\begin{gathered} S = -\iint d\tau d\tau' \, d_\sigma^+(\tau) \, \mathcal{G}_{0\sigma}^{-1}(\tau-\tau') \, d_\sigma(\tau') + \int d\tau \, U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau) \\ \mathcal{G}_{0\sigma}^{-1}(i\omega_n) = i\omega_n + \varepsilon_d - \Delta_\sigma(i\omega_n) \end{gathered}}$$

$$\Delta_\sigma = \sum_\lambda \frac{|V_\lambda|^2}{i\omega_n - \varepsilon_\lambda}$$

Spectral function of d

- Particle hole symmetric case $\epsilon_d = -\frac{U}{2}$





Kondo resonance
Abrikosov-Suhl

$T_K(U) \propto e^{-aU}$
U large

Many body effects.

- U : regular perturbation
  Δ : singular perturbation at $T=0$.

Anderson model
self energy

- $$\boxed{G_d^{-1}(i\omega_n) = i\omega_n - \varepsilon_d - \Delta(i\omega_n) - \Sigma_r(i\omega_n)}.$$

$G_{imp} = G_d$

$$\boxed{G_{imp}^{-1}(i\omega_n) = \mathcal{G}_{0d}^{-1}(i\omega_n) - \Sigma_{imp}(i\omega_n)}$$

⚠. Σ vs respect to $\mathcal{G}$ not $\frac{1}{i\omega_n - \varepsilon_d}$.

- Fermi liquid expansion at low ω.

  Anderson model is a Fermi liquid (not obvious)
  (local) = no k space

$\rightarrow$ $$\Sigma(\omega) = \left(1 - \frac{1}{Z}\right)\omega + iA\omega^2$$

$$G^{-1} = \underset{\substack{\uparrow \\ \text{flat band limit}}}{\omega + i\Gamma} - \left(1 - \frac{1}{Z}\right)\omega$$

$$G = \frac{Z}{\omega + i\underline{\Gamma Z}}$$ $\quad$ $\underline{\Gamma_{eff} = \Gamma Z(U)}$

- Level width renormalized by interaction / Z = q.p. residue
- Kondo peak is a q.p peak.