Equação de Movimento

Veremos agora porque funções de correlação como G^R:

$$G^R(rt,\vec{r}'t') = -i\,\Theta(t-t')\left\langle [\psi(\vec{r},t),\psi^\dagger(\vec{r}',t')]_{\mp}\right\rangle$$

são chamadas de "funções de Green". Diferenciando, temos:

$$i\frac{d}{dt}G^R(\vec{r}t;\vec{r}'t') = (-i)\left(i\frac{\partial}{\partial t}\Theta(t-t')\right)\left\langle [\psi(\vec{r}t),\psi^\dagger(\vec{r}t')]_{\mp}\right\rangle$$

$$+(-i)\,\Theta(t-t')\left\langle\left[i\frac{\partial\psi(\vec{r},t)}{\partial t},\psi^\dagger(\vec{r}'t')\right]_{\mp}\right\rangle$$

$$= \delta(t-t')\underbrace{\left\langle [\psi(\vec{r}),\psi^\dagger(\vec{r}')]_{\mp}\right\rangle}_{\to\ \delta(\vec{r}-\vec{r}')}$$

$$\underbrace{-i\,\Theta(t-t')\left\langle\left[i\frac{d\psi(\vec{r},t)}{dt},\psi^\dagger(\vec{r}'t')\right]_{\mp}\right\rangle}_{\equiv A^R(\vec{r}t,\vec{r}'t')}$$

$$\Rightarrow i\frac{d}{dt}G^R(\vec{r}t;\vec{r}'t') = \delta(t-t')\,\delta(r-\vec{r}') + A^R(\vec{r}t,\vec{r}'t')$$

ou, formalmente, G^R é uma função de Green:

$$\boxed{\left(i\frac{d}{dt} - A^R(\vec{r}t\vec{r}'t')(G^R)^{-1}\right)G^R(\vec{r}t\vec{r}'t') = \delta(t-t')\,\delta(\vec{r}-\vec{r}')}$$

Mas quem é $A^R(\vec{r}t,\vec{r}'t')$?

$$i\frac{d\psi(\vec{r},t)}{dt} = -[H,\psi(\vec{r})](t) = -[H_0,\psi(\vec{r})](t) - [\hat{V},\psi(\vec{r})](t)$$

onde H_0 é quadrático em $\psi(\vec{r})$ ($H_0 = \int \psi^\dagger(\vec{r}')\nabla^2_{r'}\psi(\vec{r}')\,dr'$ por exemplo)

de modo que $[H_0,\psi(\vec{r})]$, em geral, pode ser calculado e é $\propto \psi(\vec{r})$:

$$\left[i\frac{d\psi}{dt},\psi^\dagger(\vec{r}'t')\right]_{\mp} = -\underbrace{\left[[H_0,\psi(\vec{r})],\psi^\dagger(\vec{r}'t')\right]_{\mp}}_{\text{"fechado"}\ \propto\ \psi(\vec{r})} - \underbrace{\left[[\hat{V},\psi(\vec{r})],\psi^\dagger(\vec{r}'t')\right]_{\mp}}_{\text{sequência de termos}}$$

Logo, $A^R = \hat{A} G^R + D^R$ onde D^R será dado por:

$$D^R(\vec{r}t,\vec{r}'t') = -i\,\theta(t-t')\left\langle \left[-[\hat{V},\psi(\vec{r})]_-(t), \psi^\dagger(\vec{r}',t') \right]_\mp \right\rangle$$

e a questão é: $D^R(\vec{r}.t,\vec{r}'t')$ pode ser escrita em termos de funções de Green de partícula única do tipo G^R_{AB} onde $G^R_{AB}(\vec{r}t,\vec{r}'t') = -i\,\theta(t-t')\langle [\hat{A}(\vec{r},t),\hat{B}(\vec{r}',t')]_\mp\rangle$ sendo $\hat{A},\hat{B}$ operadores de um corpo? Veremos alguns casos em que isso é possível.

Antes, vejamos a transf. de Fourier da Eq. de Movimento, escritas na base $\{|\nu\rangle\}$ que diagonaliza (ou pelos menos torna quadrático) H_0:

$$H_0 = \sum_{\nu\nu'} t_{\nu'\nu}\, a^\dagger_{\nu'} a_\nu \quad \Rightarrow \quad [H_0, a_\nu] = -\sum_{\nu''} t_{\nu\nu''}\, a_{\nu''}$$

Assim:

$$G^R(\nu t;\nu' t') = -i\,\theta(t-t')\left\langle [a_\nu(t), a^\dagger_{\nu'}(t')]_\mp \right\rangle$$

$\Rightarrow$ Eq. de Movimento: $i\dfrac{d}{dt} G^R(\nu t,\nu' t') = \delta(t-t')\,\delta_{\nu\nu'} + A^R(\nu t,\nu' t')$

onde $A^R(\nu t,\nu' t') = \underbrace{-i\,\theta(t-t')\left\langle \left[[H_0,a_\nu(t)],a^\dagger_{\nu'}(t)\right]_\mp\right\rangle}_{} - i\,\theta(t-t')\left\langle\left[-[\hat{V},a_\nu],a^\dagger_{\nu'}\right]_\mp\right\rangle$

$$= \sum_{\nu''} t_{\nu\nu''}\, G^R(\nu'' t;\nu' t') + D^R(\nu t,\nu' t')$$

Logo: podemos escrever:

$$\boxed{\sum_{\nu''}\left(i\,\delta_{\nu\nu''}\frac{d}{dt} - t_{\nu\nu''}\right) G^R(\nu'' t,\nu' t') = \delta(t-t')\,\delta_{\nu\nu'} + D^R(\nu t,\nu' t')}$$

onde $\boxed{D^R(\nu t,\nu' t') = -i\,\theta(t-t')\left\langle\left[-[\hat{V},a_\nu],a^\dagger_{\nu'}\right]_\mp\right\rangle}$

Fazendo a transf de Fourier:

$$G^R(\nu\nu'\omega) = \int_{-\infty}^{\infty} d(t-t')\, e^{i\omega^+(t-t')}\, G^R(\nu\nu'(t-t'))$$

$$G^R(\nu t, \nu' t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega(t-t')}\, G^R(\nu,\nu',\omega)$$

$$\Rightarrow i\frac{d}{dt}G^R \rightarrow \underbrace{i(-i)}_{+1}\omega^+\, G^R(\nu,\nu',\omega)$$ Logo

$$\sum_{\nu''} \left(\delta_{\nu\nu''}\,\omega^+ - t_{\nu\nu''}\right) G^R(\nu'',\nu'\omega) = \delta_{\nu\nu'} + D^R(\nu\nu'\omega)$$

onde

$$\boxed{D^R(\nu\nu',\omega^+) = -i \int_{-\infty}^{\infty} d(t-t')\, e^{i\omega^+(t-t')}\, \theta(t-t')\left\langle \left[\left[-V, a_\nu(t)\right], a^+_{\nu'}\right]_{\mp} \right\rangle}$$

que deve ser calculado em cada caso.

Exemplo 0: Partículas não-interagentes $\left(H = \sum_{\nu\nu'} t_{\nu\nu'}\, a^+_{\nu'} a_\nu\right)$

É sempre possível escrever $H = \sum_\mu \varepsilon_\mu\, a^+_\mu a_\mu$ (mud. de base)

Logo: $V = 0 \Rightarrow A^R(\mu,\mu',\omega^+) = -i \int_{-\infty}^{\infty} d(t-t')\, e^{i\omega^+(t-t')}\, \theta(t-t')\left\langle \left[\left[-H_0, a_\mu\right], a^+_{\mu'}\right]\right\rangle$

sendo $[H_0, a_\mu] = -\varepsilon_\mu a_\mu \Rightarrow A^R(\mu,\mu',\omega) = +\varepsilon_\mu\, G^R(\mu,\mu',\omega)$

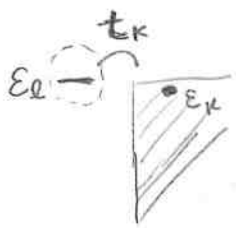
Logo, temos:

$$(\omega^+ - \varepsilon_\mu)\, G^R(\mu,\mu',\omega) = \delta_{\mu\mu'} \Rightarrow \boxed{G^R(\mu,\mu',\omega) = \frac{\delta_{\mu\mu'}}{\omega^+ - \varepsilon_\mu}}$$

Na base $\{a^+_\nu\}$, precisaríamos encontrar a matriz $\mathbb{G}^{-1}(\omega)$ cujos termos são dados por $\boxed{G^{-1}(\nu,\nu'',\omega) = \delta_{\nu\nu''}\,\omega - t_{\nu\nu''}}$ e inverter essa matriz

Exemplo 1: "Resonant level model":

nível de energia isolado acoplado a um contínuo.



$$H = H_{nível} + H_0 + H_{acop.}$$

$$H_{nível} = \varepsilon_0 c_\ell^\dagger c_\ell$$ "spinless electrons"

$$H_{band} = \sum_K \varepsilon_K c_K^\dagger c_K$$

$$H_{coup} = \sum_K t_K c_\ell^\dagger c_K + t_K^* c_K^\dagger c_\ell$$

2 operadores fermiônicos

Para calcular a função de Green de forma compacta, introduzimos a seguinte notação (Zubarev, 1960):

$$\begin{cases} \boxed{G^R_{AB}(t_1,t_2) = \langle\langle \hat{A}(t_1) : \hat{B}(t_2) \rangle\rangle} = -i\,\Theta(t_1-t_2)\langle [\hat{A}(t_1), B(t_2)]_\mp \rangle \\ G^R_{AB}(\omega) = \int_{-\infty}^{\infty} d(t_1-t_2)\, e^{i\omega^+(t_1-t_2)} \langle\langle \hat{A}(t_1) : \hat{B}(t_2) \rangle\rangle \equiv \langle\langle \hat{A} : \hat{B} \rangle\rangle_\omega \end{cases}$$

A eq. de movimiento fica na forma:

$$\boxed{\omega \langle\langle \hat{A} : \hat{B} \rangle\rangle_\omega = \langle [\hat{A}, \hat{B}]_\mp \rangle + \langle\langle [\hat{A}, \hat{H}]_- : \hat{B} \rangle\rangle}$$

Vejamos como ficam as Eqs de Movimento para as funções de Green do modelo de nível ressonante.

$$\left.\begin{aligned} G^R_{\ell\ell}(\omega) &= \langle\langle c_\ell : c_\ell^\dagger \rangle\rangle \\ G^R_{k\ell}(\omega) &= \langle\langle c_k : c_\ell^\dagger \rangle\rangle \\ G^R_{kk}(\omega) &= \langle\langle c_k : c_k^\dagger \rangle\rangle \end{aligned}\right\} \text{ função de Green dos operadores:}$$

<u>Equações de movimento:</u> (férmions) para a GF $G^R_{\ell\ell}(\omega)$:

$$\omega^+ G^R_{\ell\ell}(\omega) = \langle \{ c_\ell, c_\ell^\dagger \} \rangle + \langle\langle [c_\ell, H]_- : c_\ell^\dagger \rangle\rangle$$

comutadores:

$$[c_\ell, H]_- = [c_\ell, H_{nivel}]_- + \underbrace{\cancel{[c_\ell, H_{band}]}}_{zero} + [c_\ell, H_{coup}]$$

$$[c_\ell, H_{nivel}]: \quad c_\ell \underline{H_{nivel}} = \sum_{\ell'} \varepsilon_0 \overbrace{c_\ell c_{\ell'}^\dagger}^{\delta_{\ell\ell'} - c_{\ell'}^\dagger c_\ell} c_{\ell'} \delta_{\ell\ell'} = \sum_{\ell'} (\delta_{\ell\ell'})^2 \varepsilon_0 c_{\ell'} - \sum_{\ell'} \varepsilon_0 c_{\ell'}^\dagger \overbrace{c_\ell c_{\ell'}}^{\delta_{\ell\ell'}}$$

$$= \varepsilon_0 c_\ell + \underline{\sum_{\ell'} \delta_{\ell\ell'} \varepsilon_0 c_{\ell'}^\dagger c_{\ell'} c_\ell} = \varepsilon_0 c_\ell + H_{nivel} c_\ell$$

$$\Rightarrow \boxed{[c_\ell, H_{nivel}] = \varepsilon_0 c_\ell}$$

$$[c_\ell, H_{coup}]: \quad c_\ell H_{coup} = \sum_{k\ell'} t_k \overbrace{c_\ell c_{\ell'}^\dagger}^{\delta_{\ell\ell'} - c_{\ell'}^\dagger c_\ell} c_k \delta_{\ell\ell'} + t_k^* c_\ell c_k^\dagger c_{\ell'} \delta_{\ell\ell'}$$

$$= \sum_{k\ell'} t_k (\delta_{\ell\ell'})^2 c_k - \sum_{k\ell'} t_k c_{\ell'}^\dagger \overbrace{c_\ell c_k}^{\delta_{\ell\ell'}} + t_k^* c_k^\dagger c_{\ell'} c_\ell \delta_{\ell\ell'}$$

$$= \sum_k t_k c_k + \left[\sum_{k\ell'} \left(t_k c_{\ell'}^\dagger c_k + t_k^* c_k^\dagger c_{\ell'} \right) \delta_{\ell\ell'} \right] c_\ell$$

$$\boxed{[c_\ell, H_{coup}] = \sum_k t_k c_k}$$

$$\Rightarrow \boxed{[c_\ell, H] = \varepsilon_0 c_\ell + \sum_k t_k c_k}$$

Logo, temos:

$$\omega^+ G^R_{\ell\ell}(\omega) = 1 + \langle\langle \varepsilon_0 c_\ell : c_\ell^\dagger \rangle\rangle_\omega + \sum_k t_k \langle\langle c_k : c_\ell^\dagger \rangle\rangle_\omega$$

$$\omega^+ G^R_{\ell\ell}(\omega) = 1 + \varepsilon_0 G^R_{\ell\ell}(\omega) + \sum_k t_k G^R_{k\ell}(\omega)$$

$$\Rightarrow \boxed{(\omega^+ - \varepsilon_0) G^R_{\ell\ell}(\omega) = 1 + \sum_k t_k G^R_{k\ell}(\omega)} \quad (I) \text{ "não fechou"}$$

Eq. de movimento para $G^R_{k\ell}(\omega)$:

$$\omega^+ G^R_{k\ell}(\omega) = \overbrace{\cancel{\langle\{c_k, c_\ell^\dagger\}\rangle_\omega}}^{\text{zero}} + \langle\langle [c_k, H]_- : c_\ell^\dagger \rangle\rangle_\omega$$

Comutadores: $[c_k, H]_- = [c_k, H_{coup}] + [c_k, H_{band}] + \overbrace{\cancel{[c_k, H_{nivel}]}}^{\text{zero}}$

$[c_k, H_{coup}]$:

$$c_k H_{coup} = \sum_{k'} t_{k'}^* c_k c_{k'}^\dagger c_\ell + t_k c_k c_\ell^\dagger c_{k'}$$

$$= \sum_{k'} t_{k'}^* \delta_{kk'} c_\ell - \sum_{k'} t_{k'}^* c_{k'}^\dagger c_k c_\ell + t_k c_\ell^\dagger c_{k'} c_k$$

$$= t_k^* c_\ell + H_{coup} c_k \Rightarrow [c_k, H_{coup}] = t_k^* c_\ell$$

$[c_k, H_{band}] = \varepsilon_k c_k$ (vide $[c_\ell, H_{nivel}]$ ...)

$$\boxed{[c_k, H]_- = \varepsilon_k c_k + t_k^* c_\ell}$$ Logo

$$\omega^+ G^R_{k\ell}(\omega) = \varepsilon_k \overbrace{\langle\langle c_k : c_\ell^\dagger \rangle\rangle}^{G_{k\ell}} + t_k^* \overbrace{\langle\langle c_\ell : c_\ell^\dagger \rangle\rangle}^{G_{\ell\ell}}$$

$$\boxed{(\omega^+ - \varepsilon_k) G^R_{k\ell}(\omega) = t_k^* G^R_{\ell\ell}(\omega)} \quad (II) \text{ "fechou"}$$

$$\hookrightarrow \boxed{G^R_{k\ell}(\omega) = \frac{t_k^*}{(\omega - \varepsilon_k)} G^R_{\ell\ell}(\omega)}$$

Substituindo (II) em (I), temos:

$$(\omega^+ - \varepsilon_0)\, G^R_{\ell\ell}(\omega) = 1 + \sum_k t_k \left(\frac{t_k^*}{\omega - \varepsilon_k} \right) G_{\ell\ell}(\omega)$$

$$= 1 + \underbrace{\left(\sum_k \frac{|t_k|^2}{\omega^+ - \varepsilon_k} \right)}_{\equiv \Sigma_1(\omega)} G^R_{\ell\ell}(\omega) = 1 + \Sigma_1^R(\omega)\, G^R_{\ell\ell}(\omega)$$

$$\Rightarrow \left(\omega^+ - \varepsilon_0 - \Sigma_1^R(\omega) \right) G^R_{\ell\ell}(\omega) = 1$$

ou
$$\boxed{G^R_{\ell\ell}(\omega) = \frac{1}{(\omega^+ - \varepsilon_0 - \Sigma_1^R(\omega))}}$$

$\Sigma_1^R \rightarrow$ "auto-energia"

comparando com a funçõo de Green do nível isolado:

$$g_\ell(\omega) = \frac{1}{(\omega^+ - \varepsilon_0)} \Rightarrow \omega^+ - \varepsilon_0 = g_\ell^{-1}(\omega)$$

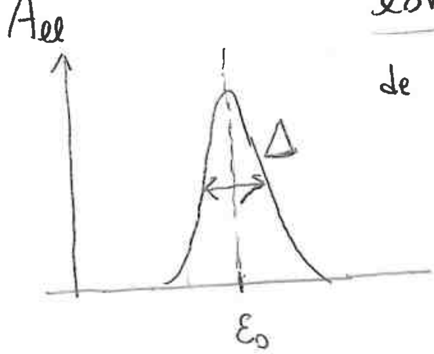
temos
$$\boxed{G^R_{\ell\ell}(\omega) = \left(g_\ell^{-1}(\omega) - \Sigma_1^R(\omega) \right)^{-1}}$$

Escrevendo $\Sigma_1^R = \Lambda(\omega) - i\Delta(\omega)$, temos que a <u>função espectral</u> de $G^R_{\ell\ell}(\omega)$ será: $A_{\ell\ell}(\omega) = -\frac{1}{\pi} \operatorname{Im} G^R_{\ell\ell}(\omega)$:

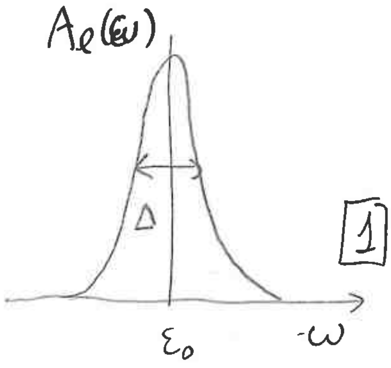
$$A_{\ell\ell}(\omega^+) = \frac{\Delta(\omega)/\pi}{(\omega^+ - \tilde{\varepsilon}_0)^2 + \Delta^2(\omega)}$$

$$\tilde{\varepsilon}_0 = \varepsilon_0 - \Lambda(\omega)$$

Se $\begin{cases} \Lambda(\omega) \equiv 0 \\ \Delta(\omega) = \Delta \end{cases}$, $A_\ell(\omega)$ é uma <u>lorentziana</u> de largura Δ.



Algumas propriedades de $A_{\ell\ell}(\omega)$



$$A_{\ell\ell}(\omega^+) = \frac{\Delta/\pi}{(\omega-\varepsilon_0)^2+\Delta^2}.$$

$\boxed{1}$. $\int_{-\infty}^{\infty} A_{\ell\ell}(\omega)\,d\omega = 1$ (normalização)

$\boxed{2}$. a $T=0$, OCUPAÇÃO MÉDIA $\boxed{\langle \hat{n}_\ell\rangle = \int_{-\infty}^{E_F} A_{\ell\ell}(\omega)\,d\omega}$ $E_F \to$ nível de Fermi do contínuo.

Prova: $\langle \hat{n}_\ell\rangle = \langle c^\dagger_\ell c_\ell\rangle = -i\,G^<_{\ell\ell}(t=t'=0)$ $\left(G^<_{\ell\ell} = +i\langle c^\dagger_\ell(t')\,c(t)\rangle\right)$

$$= -i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,G^<(\omega)\,\underbrace{e^{i\omega(0-0)}}_{1}$$

$\left(-i\,G^<_\ell(\omega) = 2\pi A_\ell(\omega)\,n_F(\omega)\right)$ TEOREMA FLUTUAÇÃO-DISSIPAÇÃO

$\left(n_F = (1+e^{\beta\omega})^{-1}\right)$

$$\boxed{\langle \hat{n}_\ell\rangle = \int_{-\infty}^{\infty} d\omega\, A_\ell(\omega)\, n_F(\omega)}$$

a $T=0$ $n_F = \Theta(\omega < E_F) \Rightarrow \boxed{\langle \hat{n}_\ell\rangle = \int_{-\infty}^{E_F} A_\ell(\omega)\,d\omega}$ $(T=0)$

$\boxed{3}$. Para $\Delta\to 0$, $\boxed{A_\ell(\omega)\to\delta(\omega-\varepsilon_0)}$

Prova: ① Se $\Sigma\to 0$ $G^R_\ell(\omega)\to g_\ell(\omega) = \dfrac{1}{\omega+i\eta-\varepsilon_0} = \mathcal{P}\left(\dfrac{1}{\omega-\varepsilon_0}\right) - i\pi\,\delta(\omega-\varepsilon_0)$

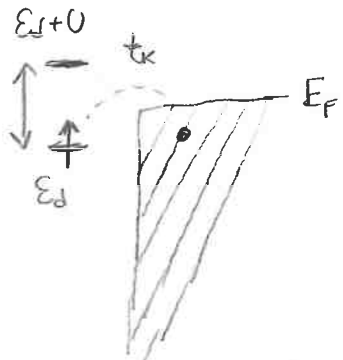
$$\Rightarrow -\frac{1}{\pi}\,\mathrm{Im}\,g_\ell(\omega) = \delta(\omega-\varepsilon_0)$$

② Isso vem da rep. da delta: $\pi\,\delta(\varepsilon-\varepsilon_\alpha) = \lim_{s\to 0^+}\dfrac{s}{(\varepsilon-\varepsilon_\alpha)^2+s^2}$

$$\Rightarrow \boxed{\lim_{\Delta\to 0}\frac{\Delta/\pi}{(\omega-\varepsilon_0)^2+\Delta^2} = \delta(\omega-\varepsilon_0)}$$

O Modelo de Anderson

Modelo de "impureza" (sistema com graus de liberdade finitos) acoplado a um contínuo de elétrons. Originalmente, o modelo foi proposto para descrever sistemas de impurezas magnéticas (níveis d incompletos) em metais. Posteriormente, foi extendido e aplicações a outros sistemas (pontos quânticos, etc.)



$\boxed{\text{Impureza}}$: nível único com interação elétron-elétron

$$H_d = \sum_\sigma \underbrace{\varepsilon_d c^\dagger_{d\sigma} c_{d\sigma}}_{\text{elétron de spin } \sigma} + \underbrace{U \hat{n}_{d\uparrow}\hat{n}_{d\downarrow}}_{\boxed{\text{interação}}} \qquad \hat{n}_{d\sigma} = c^\dagger_{d\sigma} c_{d\sigma}$$

Espaço de Hilbert da impureza:

$$|0\rangle \,, \quad |\uparrow\rangle = c^\dagger_{d\uparrow}|0\rangle \,, \quad |\downarrow\rangle = c^\dagger_{d\downarrow}|0\rangle \,, \quad |\uparrow\downarrow\rangle = c^\dagger_{d\uparrow}c^\dagger_{d\downarrow}|0\rangle$$

<u>Energias</u> (vazio)

$$\boxed{H_d|0\rangle = 0} \;; \quad \underline{H_d|\uparrow\rangle} = \varepsilon_d\big(\underbrace{c^\dagger_{d\uparrow} c_{d\uparrow}}_{\hat{n}_{d\uparrow}}|\uparrow\rangle\big) = \varepsilon_d\, c^\dagger_{d\uparrow} \underbrace{c_{d\uparrow} c^\dagger_{d\uparrow}}_{1 - c^\dagger_{d\uparrow}c_{d\uparrow}}|0\rangle$$

$$= \varepsilon_d c^\dagger_{d\uparrow}|0\rangle - 0 = \underline{\varepsilon_d|\uparrow\rangle} \quad \text{(mesmo para } |\downarrow\rangle\text{)}$$

$$H_d|\uparrow\downarrow\rangle = \varepsilon_d(\hat{n}_{d\uparrow} + \hat{n}_{d\downarrow})|\uparrow\downarrow\rangle + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}|\uparrow\downarrow\rangle$$

$$= (2\varepsilon_d|\uparrow\downarrow\rangle + U.1.1\,|\uparrow\downarrow\rangle = (2\varepsilon_d + U)|\uparrow\downarrow\rangle$$

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

Energia do estado duplamente ocupado $|\uparrow\downarrow\rangle$ maior do que a do estado simplesmente ocupado ($|\uparrow\rangle, |\downarrow\rangle$) por um valor $\underline{\varepsilon_d + U}$ ($U \to$ repulsão Coulombiana) $\to$ MODELO INTERAGENTE

Modelo de Anderson → hibridização com a banda:

$$H_{band} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}$$ → banda contínua

$$H_{hyb} = \sum_{k\sigma} t_k c^\dagger_{d\sigma} c_{k\sigma} + t^*_k c^\dagger_{k\sigma} c_{d\sigma}$$ → acoplamento impureza-banda.

$$\boxed{H_{Anderson} = H_A = H_d + H_{band} + H_{hyb}}$$

Equações de Movimento para o modelo de Anderson.

4 operadores (fermiônicos) distintos: $\underbrace{c^\dagger_{d\uparrow}, c_{d\downarrow}}_{c^\dagger_{d\sigma}}, \underbrace{c^\dagger_{k\uparrow}\ c^\dagger_{k\downarrow}}_{c^\dagger_{k\sigma}}$ → MAS modelo preserva simetria de spin S_z $(\langle n_{d\uparrow}\rangle = \langle n_{d\downarrow}\rangle)$

Eq de Movimento para $G^R_{dd\sigma}(\omega) = \langle\langle c_{d\sigma} : c^\dagger_{d\sigma}\rangle\rangle_\omega$

$$\omega^+ \langle\langle c_{d\sigma} : c^\dagger_{d\sigma}\rangle\rangle = \langle\{c_{d\sigma}, c^\dagger_{d\sigma}\}\rangle + \langle\langle [c_{d\sigma}, H_A]_- : c^\dagger_{d\sigma}\rangle\rangle$$

comutador: $[c_{d\sigma}, H_A] = [c_{d\sigma}, H_d] + [c_{d\sigma}, H_{hyb}] +$

como vimos: $[c_{d\sigma}, H_{hyb}] = \sum_k t_k c_{k\sigma}$ e $[c_{d\sigma}, \sum_{\sigma'} \varepsilon_d \hat{n}_{d\sigma'}] = \varepsilon_d c_{d\sigma}$

Fica faltando: $\bar{\sigma} = -\sigma$

$$[c_{d\sigma}, U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}] = U[c_{d\sigma}, \hat{n}_{d\sigma}\hat{n}_{d\bar{\sigma}}] = U(c_d \hat{n}_{d\sigma}\hat{n}_{d\bar{\sigma}} - \hat{n}_{d\sigma}\overset{\text{comuta.}}{\hat{n}_{d\bar{\sigma}} c_{d\sigma}})$$

$$= U\underbrace{[c_{d\sigma}, \hat{n}_{d\sigma}]}_{1.c_{d\sigma}}\hat{n}_{d\bar{\sigma}} = U c_{d\sigma}\hat{n}_{d\bar{\sigma}} \ //$$

Logo, temos:

$$[c_{d\sigma}, H_A] = \varepsilon_d c_{d\sigma} + U\hat{n}_{d\bar{\sigma}} c_{d\sigma} + \sum_k t_k c_{k\sigma} \quad \text{e}$$

$$\omega^+ G_{\underset{\sigma}{dd}}(\omega) = 1 + \varepsilon_d \langle\langle c_{d\sigma} : c^\dagger_{d\sigma} \rangle\rangle + \sum_k t_k \langle\langle c_{k\sigma} : c^\dagger_{d\sigma} \rangle\rangle$$

$$+ U \underbrace{\langle\langle \hat{n}_{d\bar{\sigma}} c_{d\sigma} : c^\dagger_{d\sigma} \rangle\rangle}_{\equiv D^R_{\sigma\sigma}(\omega)}$$

$$\omega^+ G_{\underset{\sigma}{dd}}(\omega) = 1 + \varepsilon_d G_{dd}(\omega) + \sum_k t_k G_{kd}(\omega) + U D^R(\omega)$$

$$\Rightarrow \boxed{(\omega^+ - \varepsilon_d) G_{\underset{\sigma}{dd}}(\omega) = 1 + \sum_k G_{\underset{\sigma}{kd}}(\omega) + U D^R_{\sigma\sigma}(\omega)} \quad (\mathrm{I})$$

—//—

Eq de Movimento para $G_{kd}(\omega) = \langle\langle c_{k\sigma} : c^\dagger_{d\sigma} \rangle\rangle$

$$\omega^+ \langle\langle c_{k\sigma} : c^\dagger_{d\sigma} \rangle\rangle = \underbrace{\langle \{c_{k\sigma}, c^\dagger_{d\sigma}\} \rangle}_{\text{zero}} + \langle\langle [c_{k\sigma}, H_A]_- : c^\dagger_{d\sigma} \rangle\rangle$$

comutador: $[c_{k\sigma}, H_A]_- = [c_{k\sigma}, H_{band}] + [c_{k\sigma}, H_{hyb}]_-$

$$[c_{k\sigma}, H_{band}]_- = [c_{k\sigma}, \sum_{k'} \varepsilon_{k'} n_{k'\sigma}]_- = \varepsilon_k c_{k\sigma}$$

$$[c_{k\sigma}, H_{hyb}]_- = [c_{k\sigma}, \sum_{k'} t^*_{k'} c^\dagger_{k'\sigma} c_{d\sigma}] = \sum_k t^*_k c_{d\sigma}$$

$$\omega^+ G_{\underset{\sigma}{kd}}(\omega) = \varepsilon_k \underbrace{\langle\langle c_{k\sigma} : c^\dagger_{d\sigma} \rangle\rangle}_{G_{\underset{\sigma}{kd}}(\omega)} + \sum_k t^*_k \underbrace{\langle\langle c_{d\sigma} : c^\dagger_{d\sigma} \rangle\rangle}_{G_{\underset{\sigma}{dd}}(\omega)}$$

$$\Rightarrow (\omega^+ - \varepsilon_k) G_{\underset{\sigma}{kd}}(\omega) = \sum_k t^*_k G_{\underset{\sigma}{dd}}(\omega) \Rightarrow \boxed{G_{\underset{\sigma}{kd}}(\omega) = \sum_k \frac{t^*_k}{(\omega - \varepsilon_k)} G_{\underset{\sigma}{dd}}(\omega)} \quad (\mathrm{II})$$

"fechou"?

Substituindo (II) em (I) :

$$(\omega^+ - \varepsilon_d)\, G^R_{dd\,\sigma}(\omega) = 1 + \left(\sum_k \frac{|t_k|^2}{(\omega - \varepsilon_k)} \right) G_{dd\,\sigma}(\omega) + U\, D^R_{\bar{\sigma}\sigma}(\omega)$$

$$\Rightarrow \left(\omega^+ - \varepsilon_d - \sum_k \frac{|t_k|^2}{(\omega^+ - \varepsilon_k)} \right) G^R_{dd\,(\sigma)}(\omega) = 1 + U \underline{\langle\langle n_{d\bar{\sigma}} C_{d\sigma} : C^\dagger_{d\sigma} \rangle\rangle}$$

"não fechou"

Eq. de movimento para $D^R_{\bar{\sigma}\sigma}(\omega)$?

↳ comutador $[n_{d\bar{\sigma}} C_{d\sigma}, H_A] \rightarrow$ outros termos de ordem maior...

O que fazer ?

1º opção : campo médio Escrevemos $D^R_{\bar{\sigma}\sigma}(\omega)$ na aproximação :

$$D^R_{\bar{\sigma}\sigma}(\omega) = \langle\langle n_{d\bar{\sigma}} C_{d\sigma} : C^\dagger_{d\sigma} \rangle\rangle_\omega \approx \langle n_{d\bar{\sigma}} \rangle \langle\langle C_{d\sigma} : C^\dagger_{d\sigma} \rangle\rangle_\omega = \langle n_{d\bar{\sigma}} \rangle\, G^R_{dd\,\sigma}(\omega)$$

Nesse caso $\boxed{G^{R(MF)}_{dd\,\sigma}(\omega) = \left(\omega^+ - \varepsilon_d - \Sigma^R(\omega^+) - U\langle n_{d\bar{\sigma}} \rangle \right)^{-1}}$

onde $\langle n_{d\bar{\sigma}} \rangle$ é a ocupação de spin oposto. O Hamiltoniano de uma impureza é simétrico em S_z de modo que $\langle n_{d\uparrow} \rangle = \langle n_{d\downarrow} \rangle$ MAS em campo médio podemos procurar soluções em que essa simetria é espontaneamente quebrada e $\langle n_{d\uparrow} \rangle \neq \langle n_{d\downarrow} \rangle$ (casos de muitas impurezas diluídas, por exemplo).

Nesse caso, permitindo $\langle n_{d\uparrow}\rangle \neq \langle n_{d\downarrow}\rangle$, temos:

$$G^{R(MF)}_{d\uparrow}(\omega) = \left(\omega^+ - \varepsilon_d - \Sigma^R_1(\omega^+) - U\langle n_{d\downarrow}\rangle\right)^{-1}$$

$$G^{R(MF)}_{d\downarrow}(\omega) = \left(\omega^+ - \varepsilon_d - \Sigma^R(\omega^+) - U\langle n_{d\uparrow}\rangle\right)^{-1}$$

Consideremos $\begin{cases} \Sigma^R_1(\omega^+) = \Lambda(\omega) - i\Delta(\omega) \approx \Lambda - i\Delta \quad \text{(simplicidade)} \\ \tilde{\varepsilon}_d = \varepsilon_d - \Lambda \end{cases}$

Lembrando que $\langle n_{d\sigma}\rangle = \int_{-\infty}^{\infty} d\omega\, A_{d\sigma}(\omega)\, n_F(\omega) \overset{(T=0)}{=} \int_{-\infty}^{E_F} d\omega\, A_{d\sigma}(\omega)$,

temos, para $\sigma = \uparrow$ (por exemplo):

$$-\frac{1}{\pi} G^{R(MF)}_{d\uparrow}(\omega) = \frac{\Delta/\pi}{(\omega^+ - \tilde{\varepsilon}_d - U\langle n_{d\downarrow}\rangle)^2 + \Delta^2} = A^{R(MF)}_{d\uparrow}(\omega)$$

$$\Rightarrow \begin{cases} \langle n_{d\uparrow}\rangle = \displaystyle\int_{-\infty}^{\infty} d\omega\, A_{d\uparrow}(\omega)\, n_F(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{n_F(\omega)\,\Delta\, d\omega}{(\omega - \tilde{\varepsilon}_d - U\langle n_{d\downarrow}\rangle)^2 + \Delta^2} \\ \langle n_{d\downarrow}\rangle = \displaystyle\int_{-\infty}^{\infty} d\omega\, A_{d\downarrow}(\omega)\, n_F(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{n_F(\omega)\,\Delta\, d\omega}{(\omega - \tilde{\varepsilon}_d - U\langle n_{d\uparrow}\rangle)^2 + \Delta^2} \end{cases}$$

que devem ser resolvidas de forma auto-consistente.

$\boxed{\begin{array}{l} A\ T=0: \\ (E_F = 0) \end{array}} \rightarrow \boxed{\langle n_{d\uparrow(\downarrow)}\rangle = \dfrac{\Delta}{\pi}\displaystyle\int_{-\infty}^{0} \frac{d\omega}{(\omega - \tilde{\varepsilon}_d - U\langle n_{d}\rangle)^2 + \Delta^2} = \frac{1}{2} - \frac{1}{\pi}\tan^{-1}\left(\frac{\tilde{\varepsilon} + U\langle n_{d\downarrow(\uparrow)}\rangle}{\Delta}\right)}$

(prove!)

o que leva à soluções auto-consistentes com $\langle n_{d\uparrow}\rangle \neq \langle n_{d\downarrow}\rangle$ dependendo de $\tilde{\varepsilon}_d$ ($\tilde{\varepsilon}_d = 0 \rightarrow$ energia de Fermi) (Lista 3)