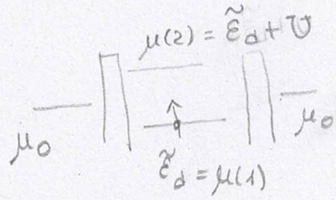
4.6. Conductance of the single impurity Anderson model

Bruus & Flensberg 10.

Wanted : $\langle \hat{I}_L \rangle = -\langle \hat{I}_R \rangle$

Start from $\hat{H}_{tot} = \hat{H}_L + \hat{H}_R + \hat{H}_{TL} + \hat{H}_{TR} + \hat{H}_D$

with
$$\begin{cases} \hat{H}_D = \sum_\sigma \tilde{\varepsilon}_d (V_g)\, \hat{d}^\dagger_\sigma \hat{d}_\sigma + \hat{U} \hat{n}_\uparrow n_\downarrow & (4.67) \\ \tilde{\varepsilon}_d = \varepsilon_d - \alpha e V_g . \end{cases}$$



and $\hat{H}_{T\alpha} = \sum_{k\sigma} \left(t_{\alpha k} c^\dagger_{\alpha\sigma} d_\sigma + t^*_{\alpha k} d^\dagger_\sigma c_{\alpha\sigma} \right)$

$\hat{H}_\alpha = \sum_{k\sigma} \varepsilon_k \hat{c}^\dagger_{\alpha k\sigma} \hat{c}_{\alpha k\sigma}$

tunneling rates

Because the single level quantum dot is also a single site quantum dot, tunneling is proportional

if the two reservoirs are assumed to have weakly dependent tunneling around the Fermi level $\mu_0 = \varepsilon_F$

As we shall see, tunneling is characterized by

$$\Gamma_\alpha(\varepsilon) = \frac{2\pi}{\hbar} \sum_{k\sigma} |t_{\alpha k}|^2 \, \delta(\varepsilon - \varepsilon_k), \quad (4.76) \text{ tunneling rate}$$

Thus it holds

$$\Gamma_\alpha \simeq \frac{2\pi |t_\alpha|^2}{\hbar} \sum_{k\sigma} \delta(\varepsilon - \varepsilon_k) = \frac{2\pi |t_\alpha|^2}{\hbar} \mathcal{D}(\varepsilon)$$

if weakly energy-dependent $t_{\alpha k}$ near μ_0

wide-band approximation

$\Rightarrow$ near μ_0 $\boxed{\Gamma_\alpha(\varepsilon) \sim \Gamma_\alpha(\mu_0) \equiv \Gamma_\alpha = \frac{2\pi |t_\alpha|^2}{\hbar} \mathcal{D}(\mu_0)}$ (4.76b)

$\Rightarrow$ $\boxed{\Gamma_L / \Gamma_R = |t_L|^2 / |t_R|^2}$ (4.77) proportional coupling

"Even-odd" basis

The relation between $\hat{H}_T$ and $\hat{I}$ suggests to perform the following transformation for bath operators

$$\begin{pmatrix} \hat{c}_{e\vec{k}\sigma} \\ \hat{c}_{o\vec{k}\sigma} \end{pmatrix} = \frac{1}{\sqrt{|t_L|^2+|t_R|^2}} \begin{pmatrix} t_L^* & t_R^* \\ -t_R & t_L \end{pmatrix} \begin{pmatrix} \hat{c}_{L\vec{k}\sigma} \\ \hat{c}_{R\vec{k}\sigma} \end{pmatrix} \qquad (4.78)$$

for each momentum $\vec{k}$ ($\Leftrightarrow$ energy E)

Inverse transformation

$$\begin{pmatrix} c_{L\vec{k}\sigma} \\ c_{R\vec{k}\sigma} \end{pmatrix} = \frac{1}{\sqrt{|t_L|^2+|t_R|^2}} \begin{pmatrix} t_L & -t_R^* \\ t_R & t_L^* \end{pmatrix} \begin{pmatrix} c_{e\vec{k}\sigma} \\ c_{o\vec{k}\sigma} \end{pmatrix} \qquad (4.78b)$$

yielding

assume for simplicity same dispersion for both leads

$$\hat{H}_{LR} = \hat{H}_L + \hat{H}_R = \sum_{\alpha\vec{k}\sigma} \varepsilon_{\alpha\vec{k}} \hat{c}^\dagger_{\alpha\vec{k}\sigma} \hat{c}_{\alpha\vec{k}\sigma} \stackrel{\downarrow}{=} \sum_{\alpha\vec{k}\sigma} \varepsilon_{\vec{k}} \hat{c}^\dagger_{\alpha\vec{k}\sigma} \hat{c}_{\alpha\vec{k}\sigma}$$

$$= \sum_{a=e,o} \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} \hat{c}^\dagger_{a\vec{k}\sigma} \hat{c}_{a\vec{k}\sigma} \qquad (4.79)$$

$\alpha = \{\alpha\vec{k}\sigma\}$

$\sqrt{T} = \sqrt{|t_L|^2+|t_R|^2}$

$$c_L^\dagger c_L = \frac{1}{T} (t_L c_e - t_R^* c_o)^\dagger (t_L c_e - t_R^* c_o)$$

$$= \frac{1}{T}\left(|t_L|^2 c_e^\dagger c_e + |t_R|^2 c_o^\dagger c_o - t_L^* t_R^* c_e^\dagger c_o - t_R t_L c_o^\dagger c_e\right)$$

$$c_R^\dagger c_R = \frac{1}{T} (t_R c_e + t_L^* c_o)^\dagger (t_R c_e + t_L^* c_o) = \frac{1}{T}\left(|t_R|^2 c_e^\dagger c_e + |t_L|^2 c_o^\dagger c_o + t_R^* t_L^* c_e^\dagger c_o + t_L t_R c_o^\dagger c_e\right)$$

(*) assume for simplicity spin-indep. tunneling amplitudes

Finally, the current operator

$$\hat{I} = \gamma \hat{I}_L - (1-\gamma)\hat{I}_R \qquad (0 \le \eta \le 1)$$

becomes with $\gamma = \frac{|t_R|^2}{|t_L|^2 + |t_R|^2} = \frac{|t_R|^2}{T^2}$

$$\boxed{\hat{I} = -\frac{ie}{\hbar} \frac{1}{\sqrt{T}} \sum_{\vec{k}\sigma} \left(t_L t_R \, c^+_{o\vec{k}\sigma} d_\sigma - t_L^* t_R^* \, d^+_\sigma c_{o\vec{k}\sigma} \right)} \quad (4.8\ldots$$

(4.58)

i.e. it only couples to "odd" operators

⇒ writing $\hat{I} = -\frac{ie}{\hbar}\left(\hat{\mathcal{L}} - \hat{\mathcal{L}}^+\right)$,

we see that simplifications occur in the even-odd basis

Start from $\mathcal{H}_{tot}$

$$\mathcal{H}_{TOT} = \underbrace{\sum_{k\sigma} \varepsilon_k \, c^+_{ek\sigma} c_{ek\sigma} + \underline{\mathcal{H}_T + \mathcal{H}_S}}_{\text{even}}$$

$$+ \underbrace{\sum_{k\sigma} \varepsilon_k \, c^+_{\sigma k\sigma} c_{\sigma k\sigma}}_{\text{odd}}$$

⇒ i) the number of charges in the odd sector does not change

ii) In the even-odd basis, the $\hat{c}_{o\vec{k}\sigma}$ and $\hat{d}_\sigma$ operators belong to separate parts of the Hamiltonian ($\rho_{tot} = \rho_{odd} \otimes \rho_{even+tun+dot}$)

↳ they represent different sorts of fermions

Consequences

i) $\Rightarrow \langle \hat{\mathcal{L}}(t)\hat{\mathcal{L}}(0)\rangle_0 = 0$

due to particle number conservation in odd sector (because $\hat{H}_T \sim \hat{c}_e$

ii) $\Rightarrow \langle c^+ d\, d^+ c\rangle_0 = \langle c^+ c\rangle\langle d d^+\rangle$

Susceptibility

$$\chi^R_{II}(t) = -\frac{i}{\hbar}\theta(t)\Big(\underbrace{\langle[\mathcal{L}(t),\mathcal{L}^+(0)]\rangle}_{I} + \underbrace{[\mathcal{L}^+(t),\mathcal{L}(0)]\rangle_0}_{II}\Big)\frac{e^2}{\hbar^2}$$

term (I)

$$\eta = \frac{|t_L|^2|t_R|^2}{|t_L|^2+|t_R|^2}$$

$$\langle[\mathcal{L}(t),\mathcal{L}^+(0)]\rangle_0 = \sum_{\vec{k}\vec{k}'}\sum_{\sigma\sigma'}\tilde{\eta}\Big[\langle c^+_{o\vec{k}\sigma}(t)\, d_\sigma(t)\, d^+_{\sigma'} c_{o\vec{k}'\sigma'}\rangle_0 - \langle d^+_{\sigma'} c_{o\vec{k}'\sigma'}\, c^+_{o\vec{k}\sigma}(t)\, d_\sigma(t)$$

$$= \sum_{\vec{k}\vec{k}'}\sum_{\sigma\sigma'}\tilde{\eta}\Big[\langle c^+_{o\vec{k}\sigma}(t)\, c_{o\vec{k}'\sigma'}(0)\rangle_0\langle d_\sigma(t) d^+_{\sigma'}\rangle_0 - \langle d^+_{\sigma'} d_\sigma(t)\rangle_0\langle c_{o\vec{k}'\sigma'}\, c^+_{o\vec{k}\sigma}(t)\rangle_0\Big]$$

$$= \sum_{\vec{k}}\sum_{\sigma}\hbar^2\tilde{\eta}\Big[G^<_{\vec{k}\sigma}(-t)\, G^>_\sigma(t) - G^>_{\vec{k}\sigma}(-t)\, G^<_\sigma(t)\Big]$$

where, in general

$$\begin{cases} G^>_{xy}(t) = -\frac{i}{\hbar}\langle\hat{c}_x(t)\hat{c}^+_y(0)\rangle & (4.82a) \text{ greater Green's function} \\ G^<_{xy}(t) = +\frac{i}{\hbar}\langle\hat{c}^+_y(0)\hat{c}_x(t)\rangle & (4.82b) \text{ lesser Green's function}\end{cases}$$

term(II) It follows from (I) upon change of sign and $t \to -t$

Frequency domain

$$\tilde{\chi}^R_{II}(\omega) = -\frac{i}{\hbar} e^2 \int_0^\infty dt\, e^{i\omega t} \sum_{\vec{k}} \sum_{\sigma} \tilde{\eta} \cdot$$

$$\cdot \left[G^<_{\vec{k}\sigma}(-t)\, G^>_{\sigma}(t) - G^>_{\vec{k}\sigma}(-t)\, G^<_{\sigma}(t) - G^<_{\vec{k}\sigma}(t)\, G^<_{\sigma}(-t) + G^>_{\vec{k}\sigma}(t)\, G^<_{\sigma}(t) \right]$$

note! $\left(G^>_{\vec{k}\sigma}(t)\right)^* = \left(-\frac{i}{\hbar} \langle c_{\vec{k}\sigma}(t)\, c^+_{\vec{k}\sigma} \rangle^* \right) = \frac{i}{\hbar} \langle c_{\vec{k}\sigma}\, c^+_{\vec{k}\sigma}(t) \rangle = -G^>_{\vec{k}\sigma}(-t)$

↳ expression in [...] is purely imaginary and odd in t

Hence

$$\mathrm{Im}\, \tilde{\chi}^R_{II}(\omega) = -\frac{e^2}{2} \frac{1}{\hbar} \int_{-\infty}^{+\infty} dt\, e^{i\omega t} \sum_{\vec{k}\sigma} \tilde{\eta} \left[\cdots \right]$$

Use

$$\int dt\, e^{i\omega t} f(t)\, g(-t) = \int \frac{d\omega'}{2\pi} \tilde{f}(\omega+\omega')\, \tilde{g}(\omega')$$

to get

$$\boxed{\begin{aligned} \mathrm{Im}\, \tilde{\chi}^R_{II}(\omega) &= -\frac{e^2}{2} \frac{1}{\hbar} \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \sum_{\vec{k}\sigma} \tilde{\eta} \cdot \\ &\cdot \left[G^>_{\sigma}(\omega') \left(G^<_{\vec{k}\sigma}(\omega'+\omega) - G^<_{\vec{k}\sigma}(\omega'-\omega) \right) - G^<_{\sigma}(\omega') \left(G^>_{\vec{k}\sigma}(\omega'+\omega) - G^>_{\vec{k}\sigma}(\omega'-\omega) \right) \right] \end{aligned}}$$

(4.83)

Relations between equilibrium Green's functions

(Bruus & Flensberg Ch. 8.3)

The Green's functions G^R, G^A and $G^<, G^>$ are defined both for equilibrium and finite voltage.

In equilibrium, they are however related to each other, as one can proof using the Lehmann representation (the representation of the eigenstates of $\hat{H}_0$, cf. e.g. Ch. 3.2)

general definitions:

In equilibrium $\langle \dots \rangle = \frac{\mathrm{Tr}\{e^{-\beta\hat{H}} \dots\}}{Z}$ or $\frac{e^{-\beta(\hat{H}-\mu_0 N)}}{Z} \dots$

$$\begin{cases} G^>_{\vec{k}\sigma}(t) = -\frac{i}{\hbar}\langle \hat{c}_{\vec{k}\sigma}(t)\, \hat{c}^+_{\vec{k}\sigma}(0)\rangle & (4.82a) \\ G^<_{\vec{k}\sigma}(t) = \frac{i}{\hbar}\langle \hat{c}^+_{\vec{k}\sigma}(0)\, \hat{c}_{\vec{k}\sigma}(t)\rangle & (4.82b) \end{cases}$$

and

$$\begin{cases} G^R_{\vec{k}\sigma}(t) = -\frac{i\theta(t)}{\hbar}\langle\{ \hat{c}_{\vec{k}\sigma}(t), \hat{c}^+_{\vec{k}\sigma}(0)\}\rangle & (4.82c) \\ G^A_{\vec{k}\sigma}(t) = \frac{i}{\hbar}\theta(-t)\langle\{ \hat{c}_{\vec{k}\sigma}(t), \hat{c}^+_{\vec{k}\sigma}(0)\}\rangle. & (4.82d) \end{cases}$$

$\Rightarrow$ $\boxed{G^R - G^A = G^> - G^<}$ (4.84) always holds

Fourier transform + Lehmann

$$\begin{cases} \tilde{G}^<_{\vec{k}\sigma}(\omega) = -\tilde{G}^>_{\vec{k}\sigma}(\omega)\, e^{-\beta(\hbar\omega-\mu_0)} & (4.85a) \text{ (in equilibrium)} \\ \tilde{G}^A_{\vec{k}\sigma}(\omega) = \left(\tilde{G}^R_{\vec{k}\sigma}(\omega)\right)^* & \text{(always)} \quad (4.85b) \end{cases}$$

Spectral function

$$\boxed{A_{\vec{k}\sigma}(\omega) = -2\,\mathrm{Im}\,\tilde{G}^R(\omega)} \quad (4.86)$$

↳ In equilibrium $\boxed{A_{\vec{k}\sigma}(\omega) = i\left(1 + e^{-\beta(\hbar\omega-\mu_0)}\right)\tilde{G}^>_{\vec{k}\sigma}(\omega)}$ (4.85c)

Note: $A_\nu(\omega)$ for noninteracting system : $\hat{H} = \sum_\nu \varepsilon_\nu \hat{c}^\dagger_\nu \hat{c}_\nu$

$$\tilde{G}^R_\nu(\omega) = -\frac{i}{\hbar}\int_{-\infty}^{+\infty} dt\, \theta(t)\, e^{i\omega t}\, e^{-i\varepsilon_\nu t/\hbar}\, e^{-\eta t}$$

$$= \frac{1}{\omega - \varepsilon_\nu/\hbar + i\eta}\,\frac{1}{\hbar}$$

$$\hookrightarrow \boxed{A_\nu(\omega) = -2\,\mathrm{Im}\,\tilde{G}^R_\nu(\omega) = \frac{2\pi}{\hbar}\,\delta(\omega - \varepsilon_\nu/\hbar)} \quad (4.86)$$

i.e., $A_\nu(\omega)$ picks up all the (single-particle) excitations

For the interacting case, $A_\nu(\omega)$ is no longer a delta-function. However, it still carries information about the system's excitations.

Note: Sum-rule for $A_\nu(\omega)$

From the relation $\langle c_\nu c^\dagger_\nu\rangle + \langle c^\dagger_\nu c_\nu\rangle = \langle c_\nu c^\dagger_\nu + c^\dagger_\nu c_\nu\rangle = 1$

$$\hookrightarrow \hbar\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi} A_\nu(\omega) = 1 \quad (4.87) \qquad \text{valid always}$$

Note: occupation of level ν

$$n_\nu = \langle c^\dagger_\nu c_\nu\rangle = -i\hbar\, G^<_\nu(t=0) = -i\hbar\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\,\tilde{G}^<_\nu(\omega)$$

$$= \hbar\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi} A_\nu(\omega) f(\omega) \quad (4.88)$$

in equilibrium

Using relation (4.84), (4.85) in (4.83)

$$\Im m\, \tilde{\chi}^{R}_{II}(\omega) = -\frac{e^2}{2}\frac{1}{\hbar}\int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}\sum_{\vec{k}\sigma}\tilde{\eta}\,.$$

$$\Big[A_{\sigma}(\omega')\, A_{\vec{k}\sigma}(\omega'+\omega)\,\underbrace{\big(f(\omega+\omega')-f(\omega')\big)}_{\frac{\partial f}{\partial \omega'}\omega} - A_{\sigma}(\omega')\, A_{\vec{k}\sigma}(\omega'-\omega)\,\underbrace{\big(f(\omega'-\omega)-f(\omega'}_{\frac{\partial f}{\partial \omega'}(-\omega)}$$

using $\omega \to 0$ and lead non interacting electrons $A_{\vec{k}\sigma}(\omega') = \frac{2\pi}{\hbar}\delta(\omega' - \varepsilon_{\vec{k}}/\hbar$

$$\hookrightarrow G = -\lim_{\omega\to 0}\frac{\Im m\,\tilde{\chi}^{R}_{II}(\omega)}{\omega} = \frac{e^2}{\hbar}\sum_{\vec{k}\sigma}\tilde{\eta}\, A_{\sigma}(\varepsilon_{\vec{k}}/\hbar)\left(-\frac{\partial f}{\partial \varepsilon_{\vec{k}}}\right)$$

Recall $\tilde{\eta} = \frac{|t_L|^2 |t_R|^2}{|t_L|^2 + |t_R|^2}$ and $\Gamma_{\alpha} = \frac{2\pi}{\hbar}|t_{\alpha}|^2 \rho(\varepsilon = \mu_0)$

$$\hookrightarrow \tilde{\eta} = \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R}\,\frac{1}{\left(\frac{2\pi}{\hbar}\rho(\mu_0)\right)}$$

Using the definition of the density of states $\rho(\varepsilon) = \sum_{\vec{k}}\delta(\varepsilon - \varepsilon_{\vec{k}})$ (per unit of spin) and $\sum_{\vec{k}} \to \int d\varepsilon\, \rho(\varepsilon)$

$$G = \frac{e^2}{\hbar}\sum_{\sigma}\tilde{\eta}\int d\varepsilon\, \rho(\varepsilon)\, A_{\sigma}(\varepsilon/\hbar)\left(-\frac{\partial f}{\partial \varepsilon}\right)$$

and finally

$$\boxed{G = e^2 \sum_{\sigma}\int \frac{d\varepsilon}{2\pi}\frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} A_{\sigma}(\varepsilon/\hbar)\left(-\frac{\partial f}{\partial \varepsilon}\right)} \qquad (4.89)$$

which is valid $\forall\, \Gamma_{L,R}$ and $\forall\, U$ ☺

Note : finite bias

As mentioned already, using non-equilibrium rather than equilibrium (

Meier & Wingreen where able to generalize (4.89) to the case of finite bias :

$$\boxed{I = e \sum_\sigma \int \frac{d\varepsilon}{2\pi} \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} A_\sigma(\varepsilon/\hbar) \left[f_L(\varepsilon) - f_R(\varepsilon) \right]} \quad (4.90)$$

where $A_\sigma(\omega) = -2 \,\mathrm{Im}\, \tilde{G}^R(\omega)$

and $\langle \cdots \rangle$ is now a nonequilibrium average $\Rightarrow A_\sigma(\omega, V)$

Wanted : $A_\sigma(\omega)$

We postpone the analysis of finite bias to the next section and focus on (4.89). I.e., we ask how the interactions + coupling to leads affect $A_\sigma(\omega)$

isolated dot $(\Gamma = 0)$ + noninteracting level

$$A_\sigma(\omega) = \frac{2\pi}{\hbar} \delta(\omega - \varepsilon_\sigma/\hbar) \equiv A^0_\sigma(\omega) \quad (4.91)$$

$$\Big\Downarrow \; U \neq 0, \; \Gamma \neq 0$$

$\boxed{A_\sigma(\omega)}$?

we need $G^R_\sigma(t) = -\frac{i}{\hbar} \theta(t) \langle \{ \hat{d}^+_\sigma(t), \hat{d}_\sigma(0) \} \rangle_0$

The equation of motion method (EOM)

$$G^R_\sigma(t) = -\frac{i}{\hbar}\,\theta(t)\,\langle\{\hat{d}_\sigma(t), \hat{d}^+_\sigma(0)\}\rangle_0 \qquad \text{dot GF}$$

to find $G^R_\sigma(t)$ one uses the EOM, where one looks at the time evolution of $G^R_\sigma(t)$. Upon taking the time derivative of both sides:

$$i\hbar\,\partial_t G^R_\sigma(t) = \delta(t)\langle\{\hat{d}_\sigma(t), \hat{d}^+_\sigma(0)\}\rangle_0 - \frac{i}{\hbar}\theta(t)\langle\{i\hbar\dot{\hat{d}}_\sigma(t), \hat{d}^+_\sigma(0)\}\rangle$$

$$= \delta(t)\langle\{\hat{d}_\sigma(t), \hat{d}^+_\sigma(0)\}\rangle_0 - \frac{i}{\hbar}\theta(t)\langle-\{[\hat{H},\hat{d}_\sigma](t), \hat{d}^+_\sigma\}\rangle_0$$

$$\dot{\hat{d}}_\sigma(t) = \frac{i}{\hbar}[\hat{H},\hat{d}_\sigma](t)$$

we need $[\hat{H},\hat{d}_\sigma]$

$$\hat{H} = \hat{H}_L + \hat{H}_R + \underbrace{\tilde{\varepsilon}_\sigma d^+_\sigma d_\sigma + U n_\uparrow n_\downarrow}_{\hat{H}_S} + \underbrace{\sum_{\vec{k}\sigma'} \sqrt{T}\,(\hat{c}^+_{e\vec{k}\sigma'}\hat{d}_{\sigma'} + \hat{d}^+_{\sigma'}\hat{c}_{e\vec{k}\sigma'})}_{\hat{H}_T}$$

$$\Rightarrow [\hat{H},\hat{d}_\sigma] = \underbrace{\tilde{\varepsilon}_\sigma d_\sigma d^+_\sigma d_\sigma}_{-\tilde{\varepsilon}_\sigma d_\sigma} + \sum_{\vec{k}\sigma'}\sqrt{T}\,\underbrace{(-\hat{c}_{e\sigma'}\delta_{\sigma\sigma'})}_{(\mathrm{I})} \underbrace{- U n_{\bar{\sigma}} d_\sigma}_{(\mathrm{II})}$$

Proof for (I): $[\hat{c}^+_{e\sigma'}\hat{d}_{\sigma'} + d^+_{\sigma'}c_{e\sigma'}, d_\sigma]$

$$= \hat{c}^+_{e\sigma'} d_{\sigma'} d_\sigma + \underbrace{d^+_{\sigma'} c_{e\sigma'} d_\sigma}_{-c_{e\sigma'}d^+_{\sigma'}d_\sigma \,=\, -c_{e\sigma'}(\delta_{\sigma\sigma'} - d_\sigma d^+_{\sigma'})} - d_\sigma c^+_{e\sigma'} d_{\sigma'} - d_\sigma d^+_{\sigma'} c_{e\sigma'}$$

$$= -\hat{c}_{e\sigma'}\delta_{\sigma\sigma'}$$

Proof for (II): $(n_\uparrow n_\downarrow d_\sigma - d_\sigma n_\uparrow n_\downarrow) \overset{\text{choose e.g. } \sigma=\downarrow \text{ and use } d^2_\sigma = 0}{=} -d_\downarrow n_\uparrow n_\downarrow = -n_\uparrow d_\downarrow(d^+_\downarrow d_\downarrow) = -n_\uparrow d_\downarrow$

$$\boxed{\begin{aligned}\Rightarrow\ i\hbar\,\partial_t G^R_\sigma(t) =\ & \delta(t)\,\langle\{\hat d_\sigma(t), \hat d^\dagger_\sigma(0)\}\rangle_0 \\ & -\frac{i}{\hbar}\,\theta(t)\,(+\tilde\varepsilon_\sigma)\,\langle\{\hat d_\sigma(t), d^\dagger_\sigma(0)\}\rangle_0 \\ & +\sum_k \sqrt{T}\,\underbrace{\left(-\frac{i}{\hbar}\,\theta(t)\right)\langle\{\hat C_{e\vec k\sigma}(t), d^\dagger_\sigma\}\rangle_0}_{g^R_{e\vec k\sigma}(t)} \leftarrow \text{mixed GF!} \\ & \underbrace{-\frac{i}{\hbar}\,\theta(t)\,\langle\{(n_{\bar\sigma}\, d_\sigma)(t), d^\dagger_\sigma\}\rangle_0}_{= D^R_\sigma(t)\ \leftarrow\ \text{higher order GF}}\, U \qquad (4.92)\end{aligned}}$$

$$\Rightarrow (i\hbar\,\partial_t - \tilde\varepsilon_\sigma)\,G^R_\sigma(t) = \delta(t)\,\overbrace{\langle\{\hat d_\sigma(t), \hat d^\dagger_\sigma(0)\}\rangle}^{=1 \text{ due to } \delta(t)} + \sum_{\vec k}\sqrt{T}\, g^R_{e\vec k\sigma}(t) + U\, D^R_\sigma(t)$$

Taking the FT ($\Rightarrow \partial_t \to -i(\omega + i\eta)$, $\delta(t) \to 1$)

$$\boxed{\begin{cases} (\hbar\omega - \tilde\varepsilon_\sigma + i\eta)\,\tilde G^R_\sigma(\omega) = \mathbb{1} + \sum_{\vec k}\sqrt{T}\,\tilde g^R_{e\vec k\sigma}(\omega) + U\,\tilde D^R_\sigma(\omega) \\[2ex] \tilde D^R_\sigma(\omega) = FT\left\{-\frac{i}{\hbar}\,\theta(t)\,\langle\{(\hat n_{\bar\sigma}\, d_\sigma)(t), d^\dagger_\sigma\}\rangle_0\right. \end{cases}} \qquad (4.93)$$

i.e. a GF of higher order is generated due to the presence of U

EOM for mixed GF

On the other hand, the mixed GF can be found from the EOM

$$i\hbar\,\partial_t\, g^R_{e\vec k\sigma}(t) = \delta(t)\,\underbrace{\langle\{\hat C_{e\vec k\sigma}(t), d^\dagger_\sigma\}\rangle}_{=0} + \varepsilon_{\vec k}\, g^R_{e\vec k\sigma}(t) + \sqrt{T}\, G^R_\sigma(t)$$

$$\Rightarrow \boxed{(\hbar\omega - \varepsilon_{\vec k} + i\eta)\,\tilde g^R_{e\vec k\sigma}(\omega) = 0 + \sqrt{T}\,\tilde G^R_\sigma(\omega)} \qquad (4.94)$$

$$\hookrightarrow \boxed{\tilde{g}^{R}_{\ell k\sigma}(\omega) = \frac{\sqrt{T}\,\tilde{G}^{R}_{\sigma}(\omega)}{\hbar\omega - \varepsilon_k + i\eta}} \qquad (4.94b)$$

Replacing in the eq. for $\tilde{G}^R_\sigma(\omega)$ in (4.93)

$$(\hbar\omega - \tilde{\varepsilon}_\sigma + i\eta)\,\tilde{G}^R_\sigma(\omega) = \mathbb{1} + T\,\tilde{G}^R_\sigma(\omega)\sum_{\vec{k}} \frac{1}{\hbar\omega - \varepsilon_k + i\eta} + U\tilde{D}^R_\sigma(\omega)$$

Define the <u>self-energy</u>

$$\Sigma^R(\omega) \equiv \underbrace{T}_{T = |t_L|^2 + |t_R|^2} \sum_{\vec{k}} \frac{1}{\hbar\omega - \varepsilon_k + i\eta} = T\int d\varepsilon \frac{\mathcal{D}(\varepsilon)}{\hbar\omega - \varepsilon + i\eta} \qquad (4.95)$$

to find the still exact expression

$$\boxed{\tilde{G}^R_\sigma(\omega) = \frac{\mathbb{1}}{\hbar\omega - \tilde{\varepsilon}_\sigma - \Sigma^R(\omega) + i\eta} + U\frac{\tilde{D}^R_\sigma(\omega)}{\hbar\omega - \tilde{\varepsilon}_\sigma - \Sigma^R(\omega) + i\eta}} \qquad (4.96)$$

self-energy due to coupling to leads

<u>note</u>: <u>wide band limit : $\mathcal{D}(\varepsilon) \sim \mathcal{D}(\mu_0)$</u>

$$\Sigma^R(\omega) \simeq T\mathcal{D}(\mu_0)\int d\varepsilon \frac{1}{\hbar\omega - \varepsilon + i\eta} = \frac{\hbar\Gamma}{2\pi}\int \frac{d\varepsilon}{\hbar\omega - \varepsilon + i\eta} \qquad (4.95b)$$

$$\Gamma = \frac{2\pi}{\hbar}T\mathcal{D}(\mu_0) = \Gamma_L + \Gamma_R$$

The function $\Sigma^R(\omega)$ is our first encounter with the concept of <u>self-energy</u>! It describes the effects of the reservoirs on the reduced dynamics,

To Eq. (4.95b) : $\dfrac{1}{\hbar\omega - \varepsilon + i\eta} = \mathcal{P}\left(\dfrac{1}{\hbar\omega - \varepsilon}\right) - i\pi\,\delta(\hbar\omega - \varepsilon)$

$$\hookrightarrow \boxed{\Sigma^R(\omega) = \frac{\hbar\Gamma}{2\pi}\mathcal{P}\int \frac{d\varepsilon}{\hbar\omega - \varepsilon + i\eta} + (-i)\frac{\hbar\Gamma}{2} = -i\frac{\hbar\Gamma}{2}} \qquad (4.95c)$$

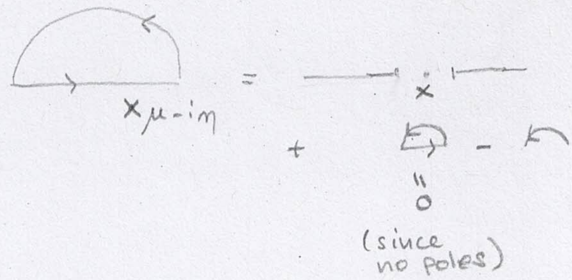
purely imaginary

Proof of (4.95b) Evaluation of the principal part integral

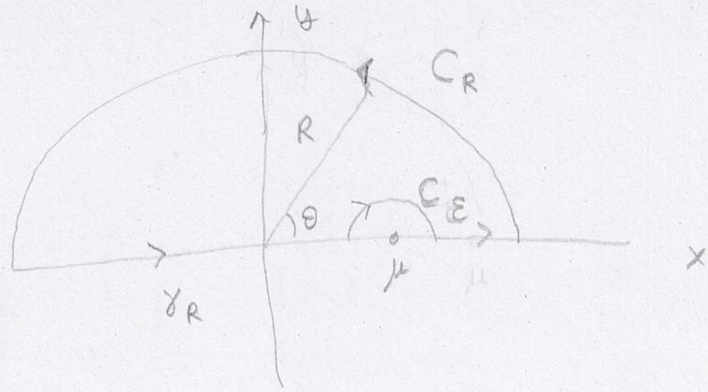
$$P\int dx \frac{1}{x-\mu+i\eta} \equiv \operatorname{Re} \lim_{\eta\to 0} \int_{-\infty}^{\infty} dx \frac{1}{x-\mu+i\eta}$$

↳ pole in the lowest half plane

Use the following contour



↳



$$\lim_{\eta\to 0}\left[\lim_{R\to\infty}\lim_{\varepsilon\to 0}\left(\int_{-R}^{\mu-\varepsilon} dx \frac{1}{x-\mu+i\eta} + \int_{\mu+\varepsilon}^{R} dx \frac{1}{x-\mu+i\eta}\right)\right.$$

$$\left. + \lim_{R\to\infty}\int_0^\pi d\theta\, iRe^{i\theta}\underbrace{\frac{1}{Re^{i\theta}-\mu+i\eta}}_{0 \text{ when } R\to\infty} + \underbrace{\lim_{\varepsilon\to 0}\int_\pi^0 i\,d\theta}_{-i\pi}\right]$$

$x = Re^{i\theta}$

$dx = iRe^{i\theta}d\theta$

$\bar{x} = \mu + \varepsilon e^{i\theta}$

$d\bar{x} = \varepsilon i e^{i\theta} d\theta$

$\frac{d\bar{x}}{\bar{x}} = i\,d\theta$

$\Rightarrow P\left(\int dx \frac{1}{x-\mu+i\eta}\right) = 0 \quad , \quad \operatorname{Im}\int dx \frac{1}{x-\mu+i\eta} = -i\pi$

it can also nicely be seen
by adding a Lorenzian convergence function $\frac{W^2}{W^2+\omega^2}$ and after $W\to\infty$

Note: Eq. (4.96) is still exact.

However, knowledge of $\tilde{G}^R$ also involves knowledge of $\tilde{D}^R$.

If we apply the EOM to $D^R(t)$, we generate higher order GF, including higher order mixed GF.

$\leadsto \infty$ hierarchy of equations ☹

Note: If $U=0$ the term containing $\tilde{D}^R_\sigma$ does not contribute

$$\boxed{\tilde{G}^R_\sigma(\omega) = \frac{1}{\hbar\omega - \tilde{\varepsilon}_\sigma - \Sigma^R(\omega) + i\eta}} \qquad (4.97) \qquad \underline{U=0}$$

Further, in the wide-band limit

$$\mathrm{Re}\,\Sigma^R(\omega) = 0, \qquad \mathrm{Im}\,\Sigma^R(\omega) = -\hbar\Gamma/2 \qquad (4.98)$$

$$\hookrightarrow \boxed{A_\sigma(\omega) = -2\,\mathrm{Im}\,\tilde{G}^R_\sigma(\omega) = \frac{\hbar\Gamma}{(\hbar\omega - \tilde{\varepsilon}_\sigma)^2 + (\hbar\Gamma/2)^2}} \qquad (4.99)$$

which has the same form as the resonance shape for the double barrier in the limit $T_1, T_2 \ll 1$ (cf. (4.57))

The final result for G in the noninteracting case is thus (again)

$$\boxed{G = e^2 \sum_\sigma \int \frac{d\varepsilon}{2\pi} \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} \frac{\hbar\Gamma}{(\varepsilon - \tilde{\varepsilon}_\sigma)^2 + (\hbar\Gamma/2)^2} \left(-\frac{\partial f}{\partial \varepsilon}\right)} \qquad (4.100)$$

EOM for $D^R(t)$

In order to describe correlation effects we need to include the effects of $U\tilde{D}^R$, at least in approximate form

↳ we iterate the EOM one step further and look at the eqs. for D^R

$$i\hbar\,\partial_t D^R_\sigma(t) = \delta(t)\,\langle\{(\hat{n}_{\bar\sigma}\hat{d}_\sigma)(t), \hat{d}^+_\sigma\}\rangle_0$$

$$-\frac{i}{\hbar}\,\theta(t)\,\langle\{-[\hat{H}_{tot}, \hat{n}_{\bar\sigma}\hat{d}_\sigma](t), \hat{d}^+_\sigma\}\rangle_0 \qquad (4.101)$$

The commutator in the last term yields two terms

$$[\hat{H}_{tot}, \hat{n}_{\bar\sigma}\hat{d}_\sigma] = [\hat{H}_S, \hat{n}_{\bar\sigma}\hat{d}_\sigma] + [\hat{H}_T, \hat{n}_{\bar\sigma}\hat{d}_\sigma]$$

with

$$[\hat{H}_S, \hat{n}_{\bar\sigma}\hat{d}_\sigma] = \hat{n}_{\bar\sigma}[\hat{H}_S, \hat{d}_\sigma] = (-\varepsilon_{d\sigma} - U)\,\hat{n}_{\bar\sigma}\hat{d}_\sigma$$

and

$$[\hat{H}_T, \hat{n}_{\bar\sigma}\hat{d}_\sigma] = \underbrace{-\sqrt{T}\,\hat{n}_{\bar\sigma}\sum_k \hat{c}_{ek\sigma}}_{\substack{\text{generates new higher order}\\ \text{mixed GF } h^R_{k\sigma}}} + \underbrace{\sum_k \sqrt{T}\,(\hat{c}^+_{ek\bar\sigma}\hat{d}_{\bar\sigma} - \hat{d}^+_{\bar\sigma}\hat{c}_{ek\bar\sigma})\hat{d}_\sigma}_{\substack{\text{generates mixed term which}\\ \text{couples to lead electrons}\\ \text{of opposite spin)}\\ \text{↳ Kondo physics}}}$$

here

$$\boxed{h^R_{ek\sigma}(t) \equiv -\frac{i}{\hbar}\,\theta(t)\,\langle\{(\hat{n}_{\bar\sigma}\hat{c}_{ek\sigma})(t), \hat{d}^+_\sigma\}\rangle_0 \qquad (4.102)}$$

<u>note</u>: h^R is similar to D^R upon replacement $\hat{c}_{ek\sigma} \to \hat{d}_\sigma$

EOM for $h^R(t)$

Similarly to what we did for $g^R(t)$, we look at the EOM for h

As usual, we need

$$[\hat{H}_{tot}, \hat{m}_{\bar{\sigma}} \hat{c}_{e\vec{k}\sigma}] = -\varepsilon_k \hat{c}_{e\vec{k}\sigma} + [\hat{H}_T, \hat{c}_{e\vec{k}\sigma}]$$

and

$$[\hat{H}_T, \hat{c}_{e\vec{k}\sigma}] = \hat{m}_{\bar{\sigma}} [\hat{H}_T, \hat{c}_{e\vec{k}\sigma}] + [\hat{H}_T, \hat{m}_{\bar{\sigma}}] \hat{c}_{e\vec{k}\sigma}$$

$$= -\sqrt{T}\, \hat{m}_{\bar{\sigma}} \hat{c}_{e\vec{k}\sigma} + \sum_{\vec{k}} \sqrt{T} (\hat{c}^{+}_{e\vec{k}\bar{\sigma}} \hat{d}_{\bar{\sigma}} - d^{+}_{\bar{\sigma}} \hat{c}_{e\vec{k}\bar{\sigma}}) \hat{c}_{e\vec{k}\sigma}$$

spin-flip processes

2) neglecting spin-flip processes in EOM for D^R and h^R the equations close

We get

$$\begin{cases} (i\hbar \partial_t - \tilde{\varepsilon}_\sigma - U) D^R_\sigma(t) = \delta(t) \langle \hat{m}_{\bar{\sigma}} \rangle + \sum_{\vec{k}} \sqrt{T}\, h^R_{\vec{k}\sigma}(t) \\ (i\hbar \partial_t - \varepsilon_{\vec{k}\sigma}) h^R_{e\vec{k}\sigma}(t) = \sqrt{T}\, D^R_\sigma(t) \end{cases} \qquad (4.103)$$

↳ after solving for $h^R_{\vec{k}\sigma}$ and summing over $\vec{k}$, one gets upon FT

$$\boxed{\tilde{D}^R_\sigma(\omega) = \frac{\langle \bar{m}_\sigma \rangle}{\hbar\omega - \tilde{\varepsilon}_\sigma - U - \Sigma^R(\omega)}} \qquad (4.104)$$

$$\tilde{G}^R_\sigma(\omega) = \frac{1}{\hbar\omega - \tilde{\varepsilon}_\sigma - \Sigma^R(\omega)}\left[1 + \frac{U\langle\hat{n}_{\bar{\sigma}}\rangle_0}{\hbar\omega - (\tilde{\varepsilon}_\sigma + U) - \Sigma^R(\omega)}\right]$$

Decompose second term in simple fractions

$$U\langle\hat{n}_{\bar{\sigma}}\rangle_0 \frac{1}{\hbar\omega - \tilde{\varepsilon}_\sigma - \Sigma^R(\omega)} \frac{1}{\hbar\omega - (\tilde{\varepsilon}_\sigma + U) - \Sigma^R(\omega)} =$$

$$U\langle\hat{n}_{\bar{\sigma}}\rangle_0 \left(\frac{A}{\hbar\omega - \tilde{\varepsilon}_\sigma - \Sigma^R(\omega)} + \frac{B}{\hbar\omega - (\tilde{\varepsilon}_\sigma + U) - \Sigma^R(\omega)}\right)$$

$$= U\langle\hat{n}_{\bar{\sigma}}\rangle_0 \frac{(A+B)(\hbar\omega - \tilde{\varepsilon}_\sigma - \Sigma_R) - AU}{(\hbar\omega - \tilde{\varepsilon}_\sigma - \Sigma^R)(\hbar\omega - (\varepsilon_\sigma + U) - \Sigma^R)}$$

$\hookrightarrow \; A = -\frac{1}{U}, \quad B = \frac{1}{U}$

$$\hookrightarrow \; \boxed{\tilde{G}^R_\sigma(\omega) = \frac{1 - \langle\hat{n}_{\bar{\sigma}}\rangle_0}{\hbar\omega - \tilde{\varepsilon}_\sigma - \Sigma^R(\omega)} + \frac{\langle\hat{n}_{\bar{\sigma}}\rangle_0}{\hbar\omega - (\tilde{\varepsilon}_\sigma + U) - \Sigma^R(\omega)}} \quad (4.105)$$

The spectral function is correspondingly

4.8

$$\boxed{A_\sigma(\omega) = \frac{\hbar\Gamma\,(1 - \langle \hat{n}_{\bar\sigma}\rangle)}{(\hbar\omega - \tilde{\varepsilon}_\sigma)^2 + (\hbar\Gamma/2)^2} + \frac{\langle \hat{n}_{\bar\sigma}\rangle\, \hbar\Gamma}{(\hbar\omega - \tilde{\varepsilon}_\sigma - U)^2 + (\hbar\Gamma/2)^2}} \quad (4.106)$$

From which the conductance G follows: $G = e^2 \sum_\sigma \int \frac{d\varepsilon}{2\pi} \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} A_\sigma\left(\frac{\varepsilon}{\hbar}\right)\left(-\frac{\partial f}{\partial \varepsilon}\right)$

peaked around μ_0

We notice that, with $\tilde{\varepsilon}_\sigma = \tilde{\varepsilon}_d = \tilde{\varepsilon}_d(V_g) = \varepsilon_d - \alpha e V_g$

$$\tilde{\varepsilon}_d = \mu(1) = E_1 - E_0 \quad - \alpha e V_g$$

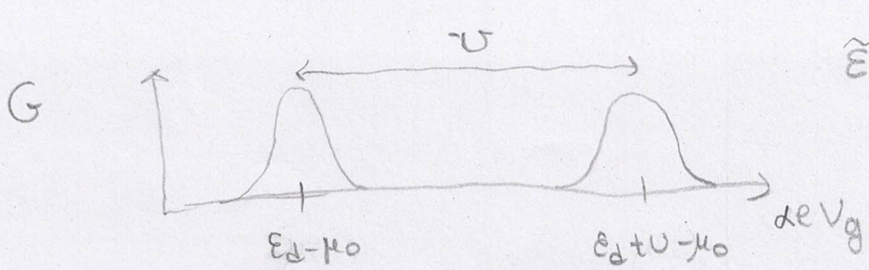
$$\tilde{\varepsilon}_d + U = \mu(2) = E_2 - E_1 \quad - \alpha e V_g$$

i.e., the first term in (4.106) represents the contribution to G from adding an electron σ to the dot if that was empty $\Rightarrow \langle \hat{n}_{\bar\sigma}\rangle = 0$;

the second term is the contribution of adding σ if already $\bar\sigma$ was present

The occupations $\langle \hat{n}_\sigma\rangle$, $\langle \hat{n}_{\bar\sigma}\rangle$ depend on the gate voltage

$$\tilde{\varepsilon}_d(V_g) = \varepsilon_d - \alpha e V_g$$



Coulomb peaks at $\mu(1) \sim \mu_0 \Rightarrow \varepsilon_d - \mu_0 = \alpha e V_g$

$\mu(2) \sim \mu_0 \Rightarrow \varepsilon_d + U - \mu_0 = \alpha e V_g$

~~Note:~~ The occupations $\langle \hat{n}_\sigma \rangle$, $\langle \hat{n}_{\bar{\sigma}} \rangle$ are not known,

These and have to be found self-consistently according to Eq. (4.85), which relates the spectral function to $\tilde{G}$

$$A_\sigma(\omega) = i\left(1 + e^{-\beta(\hbar\omega - \mu_0)}\right) \tilde{G}^>_\sigma(\omega)$$

$$\hookrightarrow \quad \tilde{G}^>_\sigma(\omega) = -i \frac{A_\sigma(\omega)}{1 + e^{-\beta(\hbar\omega - \mu_0)}}$$

Further

$$G^>_\sigma(t) = -\frac{i}{\hbar} \langle d_\sigma(t)\, d^+_\sigma(0) \rangle$$

$$1 - \langle n_\sigma \rangle = \frac{\hbar}{-i} G^>_\sigma(0) = \frac{\hbar}{-i} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \tilde{G}^>_\sigma(\omega)$$

$$= \hbar \int \frac{d\omega}{2\pi} A_\sigma(\omega) \frac{1}{1 + e^{-\beta(\hbar\omega - \mu_0)}}$$

$$\hookrightarrow \langle \hat{n}_\sigma \rangle = 1 - \hbar \int \frac{d\omega}{2\pi} A_\sigma(\omega) \frac{1}{1 + e^{-\beta(\hbar\omega - \mu_0)}}$$

$$= \hbar \int \frac{d\omega}{2\pi} A_\sigma(\omega) \left[1 - \frac{1}{1 + e^{-\beta(\hbar\omega - \mu_0)}} \right]$$

$$1 = \hbar \int \frac{d\omega}{2\pi} A_\sigma(\omega)$$

$$\hookrightarrow \boxed{\langle \hat{n}_\sigma \rangle = \hbar \int \frac{d\omega}{2\pi} A_\sigma(\omega) f(\hbar\omega)} \qquad (4.107)$$

cf. also (4.88)

↳ <u>self-consistent solution for $\langle \hat{n}_\sigma \rangle$</u>

Consider $\varepsilon_\uparrow = \varepsilon_\downarrow = \varepsilon_d \Rightarrow \langle \hat{n}_\sigma \rangle = \langle \hat{n}_{\bar{\sigma}} \rangle$

↳ $$\langle \hat{n}_\sigma \rangle = \hbar \int \frac{d\omega}{2\pi} A_\sigma(\omega) f(\omega)$$

$$= \hbar \int \frac{d\omega}{2\pi} f(\omega) \left[\frac{\hbar\Gamma (1 - \langle \hat{n}_\sigma \rangle)}{(\hbar\omega - \varepsilon_\sigma)^2 + (\hbar\Gamma/2)^2} + \frac{\langle \hat{n}_\sigma \rangle \hbar\Gamma}{(\hbar\omega - (\varepsilon_\sigma + U))^2 + (\hbar\Gamma/2)^2} \right]$$

$\langle \hat{n}_{\bar{\sigma}} \rangle = \langle \hat{n}_\sigma \rangle$

we introduce

$$n_0 \equiv \hbar \int \frac{d\omega}{2\pi} f(\omega) \frac{\hbar\Gamma}{(\hbar\omega - \varepsilon_\sigma)^2 + (\hbar\Gamma/2)^2}, \qquad (4.108a)$$

$$n_U \equiv \hbar \int \frac{d\omega}{2\pi} f(\omega) \frac{\hbar\Gamma}{(\hbar\omega - (\varepsilon_\sigma + U))^2 + (\hbar\Gamma/2)^2} \qquad (4.108b)$$

↳ $$\langle \hat{n}_\sigma \rangle = (1 - \langle \hat{n}_\sigma \rangle) n_0 + \langle \hat{n}_\sigma \rangle n_U$$

↳ $$\boxed{\langle \hat{n}_\sigma \rangle = \frac{n_0}{1 + n_0 - n_U}} \qquad (4.109)$$

1st limiting case for the conductance : T=0 (exercise)

i) $\boxed{T=0}$ $\Rightarrow$ $\underline{\underline{U, \Gamma > T}}$ (but still U not too large due to the truncation of the EOM)

The functions n_0, n_U in (4.108) can be evaluated in analytic form:

$$\int_{-\infty}^{x_0} dx \frac{1}{x^2+a^2} = \frac{1}{a}\int \frac{dx}{a} \frac{1}{\frac{x^2}{a^2}+1} = \frac{1}{a}\left[\arctan \frac{x_0}{a} + \frac{\pi}{2}\right]$$

$$\hookrightarrow n_0 = \int^{\mu_0} \hbar \frac{d\omega}{2\pi} \frac{\hbar\Gamma}{(\hbar\omega - \tilde{\varepsilon}_d)^2 + (\hbar\Gamma/2)^2}$$

$$= \int^{\mu_0-\varepsilon_d} \frac{dx}{2\pi} \frac{\hbar\Gamma}{x^2 + (\hbar\Gamma/2)^2} = \frac{1}{\pi} \arctan\left(\frac{x}{\hbar\Gamma/2}\right)\Bigg|_{-\infty}^{\mu_0-\varepsilon_d}$$

$x = \hbar\omega - \varepsilon_d$
$dx = \hbar d\omega$

$$= \frac{1}{\pi}\left[\frac{\pi}{2} - \arctan \frac{2(\tilde{\varepsilon}_d - \mu_0)}{\hbar\Gamma}\right]$$

$$\hookrightarrow \boxed{n_0 = \frac{1}{2} - \frac{1}{\pi}\arctan\frac{2(\tilde{\varepsilon}_d-\mu_0)}{\hbar\Gamma}} \quad (4.110a) \quad \text{at } T=0$$

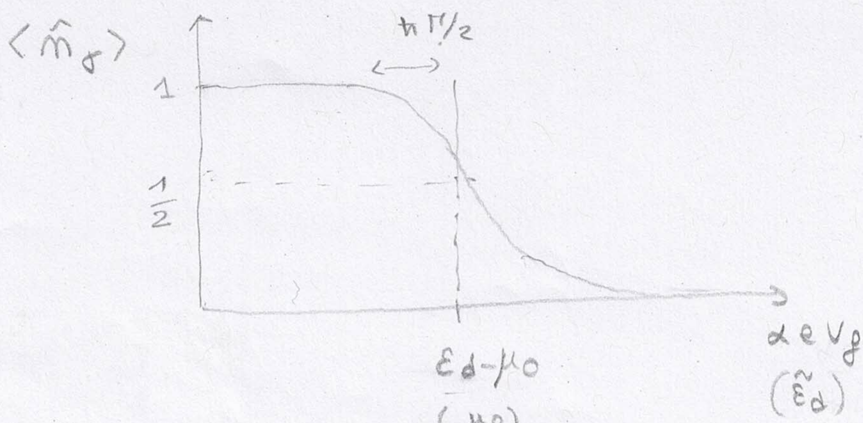
similarly

$$\boxed{n_U = \frac{1}{2} - \frac{1}{\pi}\arctan\frac{2(\tilde{\varepsilon}_d-\mu_0+U)}{\hbar\Gamma}} \quad (4.110b)$$

The weights n_0, n_U depend on V_g as well as on U:

$\underline{U=0}$ $\Rightarrow$ $n_0 = n_U \Rightarrow \langle \hat{n}_\sigma \rangle = n_0$

further $n_0 = \frac{1}{2} - \frac{1}{\pi} \arctan \frac{2(\tilde{\varepsilon}_d - \mu_0)}{\hbar\Gamma} = \begin{cases} \sim 1 & \tilde{\varepsilon}_d \ll \mu_0 \\ \sim \frac{1}{2} & \tilde{\varepsilon}_d = \mu_0 \\ \sim 0 & \tilde{\varepsilon}_d \gg \mu_0 \end{cases}$



with $\tilde{\varepsilon}_d = \varepsilon_d - \alpha e V_g$

$U=0, T=0$

similar to Fermi function but Γ broadening!

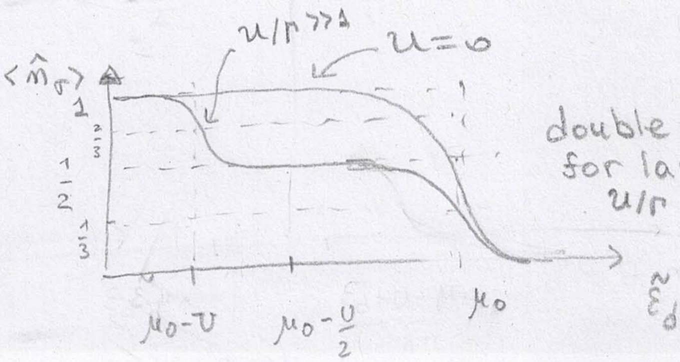
$\underline{U \neq 0}$, $\langle \hat{n}_\sigma \rangle = \frac{n_0}{1 + n_0 - n_U}$

$n_0 = \frac{1}{2} - \frac{1}{\pi} \arctan \frac{2(\tilde{\varepsilon}_d - \mu_0)}{\hbar\Gamma}$ it behaves as above

$n_U = \frac{1}{2} - \frac{1}{\pi} \arctan \frac{2(\tilde{\varepsilon}_d - \mu_0 + U)}{\hbar\Gamma} = \begin{cases} \sim 1 & \tilde{\varepsilon}_d + U \ll \mu_0 \\ \frac{1}{2} - \frac{1}{\pi} \arctan \frac{2U}{\hbar\Gamma}, & \tilde{\varepsilon}_d = \mu_0 \\ \frac{1}{2}, & \tilde{\varepsilon}_d + U \sim \mu_0 \\ \sim 0 & \tilde{\varepsilon}_d + U \gg \mu_0 \end{cases}$

$\hookrightarrow n_0 = n_U$ when $\tilde{\varepsilon}_d - \mu_0 = -\frac{U}{2}$

$\langle n_\sigma \rangle \simeq \begin{cases} 1 & \tilde{\varepsilon}_d \ll \mu_0 - U \\ \dfrac{\frac{1}{2} + \frac{1}{\pi} \arctan \frac{2U}{\hbar\Gamma}}{1 + \frac{1}{\pi} \arctan \frac{2U}{\hbar\Gamma}} & \tilde{\varepsilon}_d = \mu_0 - U \\ 1/2 & \tilde{\varepsilon}_d = \mu_0 - \frac{U}{2} \\ \dfrac{1/2}{1 + 1/\pi \arctan \frac{2U}{\hbar\Gamma}}, & \tilde{\varepsilon}_d = \mu_0 \\ \sim 0 & \tilde{\varepsilon}_d \gg \mu_0 \end{cases}$



double-step for large U/Γ

height and width of conductance peaks at T=0?

From the conductance formula (4.89) it follows

$$G = e^2 \sum_\sigma \int \frac{d\varepsilon}{2\pi} \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} A_\sigma(\varepsilon/\hbar) \left(-\frac{\partial f}{\partial \varepsilon}\right)$$

$$\hookrightarrow \boxed{G = \frac{e^2}{2\pi} \sum_\sigma \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} A_\sigma(\mu_0/\hbar) \quad \text{at } T=0 \quad (4.111)}$$

Further, from (4.106) (with $\langle \hat{n}_\sigma \rangle = \langle \hat{n}_{\bar{\sigma}} \rangle$), $\varepsilon_\sigma = \tilde{\varepsilon}_d$

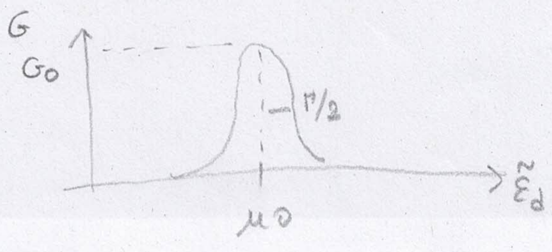
$$A_\sigma(\mu_0/\hbar) = \frac{\hbar\Gamma \,(1 - \langle \hat{n}_\sigma \rangle)}{(\mu_0 - \tilde{\varepsilon}_d)^2 + (\hbar\Gamma/2)^2} + \frac{\langle \hat{n}_\sigma \rangle \hbar\Gamma}{(\mu_0 - \tilde{\varepsilon}_d - U)^2 + \left(\frac{\hbar\Gamma}{2}\right)^2} \quad (4.112)$$

and

$$\langle \hat{n}_\sigma \rangle = \frac{n_0}{1 + n_0 - n_U}$$

with n_0, n_U given in Eqs. (4.110a), (4.110b)

$\underline{U=0}$ $\quad A_\sigma(\mu_0/\hbar) = \dfrac{\hbar\Gamma}{(\mu_0 - \tilde{\varepsilon}_d) + (\Gamma\hbar/2)^2}$, $\quad G(\tilde{\varepsilon}_d = \mu_0) = 2\dfrac{e^2}{h} \, 4 \cdot \dfrac{\Gamma_L \Gamma_R}{(\Gamma_L + \Gamma_R)}$



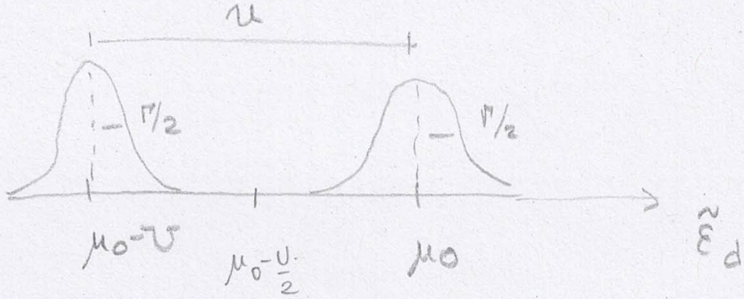
max conductance of $\frac{2e^2}{h} = G_0$

for $\Gamma_L = \Gamma_R = \frac{\Gamma}{2}$ (symmetric barriers)

$\mathcal{U} \neq 0$

i) Two peaks, each of width Γ start to develop as U grow

↳ they become distinguishable when $\mathcal{U} > \Gamma$



ii) Further, their <u>height</u> also depends on $\mathcal{U}$

We find

$$G(\tilde{\varepsilon}_d = \mu_0 - U) = \frac{2e^2}{h} \frac{\Gamma_L \Gamma_R}{(\Gamma_L + \Gamma_R)^2} \left[4 \langle \hat{m}_\sigma \rangle + \frac{4(1 - \langle \hat{m}_\sigma \rangle)(\frac{\hbar\Gamma}{2})^2}{U^2 + (\hbar\Gamma/2)^2} \right.$$

$$\xrightarrow[\frac{\mathcal{U}}{\Gamma} \gg 1]{=} \frac{2e^2}{h} \frac{4\Gamma_L\Gamma_R}{(\Gamma_L+\Gamma_R)^2} \underset{\text{check}}{\frac{2}{3}} = \underset{\text{symmetric case}}{\frac{2}{3} \cdot \frac{2e^2}{h}}$$

$$G(\tilde{\varepsilon}_d = \mu_0) = \frac{2e^2}{h} \frac{\Gamma_L\Gamma_R}{(\Gamma_L+\Gamma_R)^2} \left[4(1 - \langle \hat{m}_\sigma \rangle + \frac{4\langle \hat{m}_\sigma \rangle (\frac{\hbar\Gamma}{2})^2}{U^2 + (\hbar\Gamma/2)^2} \right]$$

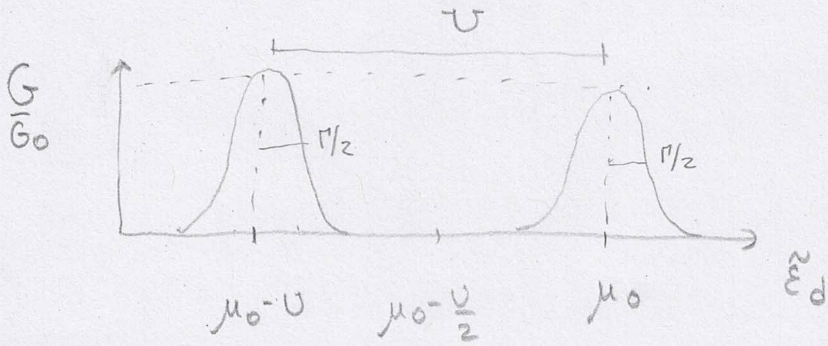
$$\underset{\frac{\mathcal{U}}{\Gamma} \gg 1}{\hookrightarrow} \frac{2e^2}{h} \frac{\Gamma_L\Gamma_R 4}{(\Gamma_L+\Gamma_R)^2} \underbrace{\left(1 - \frac{1}{3}\right)}_{\frac{2}{3}} = \underset{\text{symmetric case}}{\frac{2}{3} \frac{2e^2}{h}}$$

$$\tilde{G}\left(\tilde{\varepsilon}_d = \mu_0 - \frac{U}{2}\right) = \frac{2e^2}{h} \frac{\Gamma_L\Gamma_R 4}{(\Gamma_L+\Gamma_R)^2} \left[2 \cdot \frac{1}{2} \frac{(\hbar\Gamma/2)^2}{(U/2)^2 + (\hbar\Gamma/2)^2} \right] \xrightarrow[\text{if } \mathcal{U}/\Gamma \gg 1]{} 0$$

Summary: $T=0$ (and still $\frac{U}{\Gamma}$ not too large)

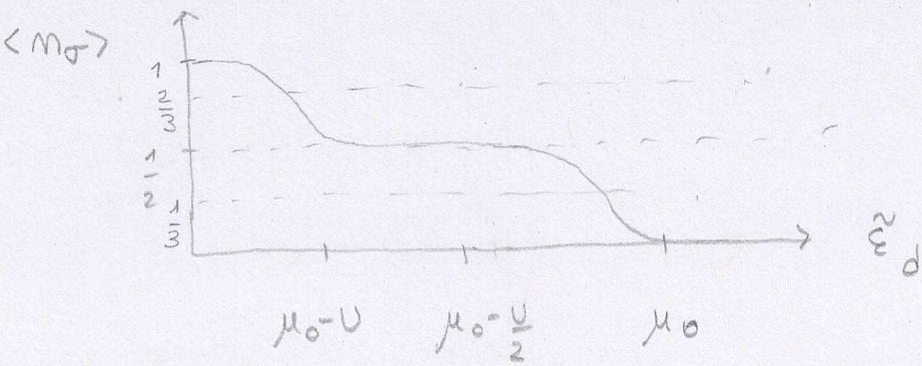
$G_0 = \frac{2e^2}{h}$

$U \neq 0$



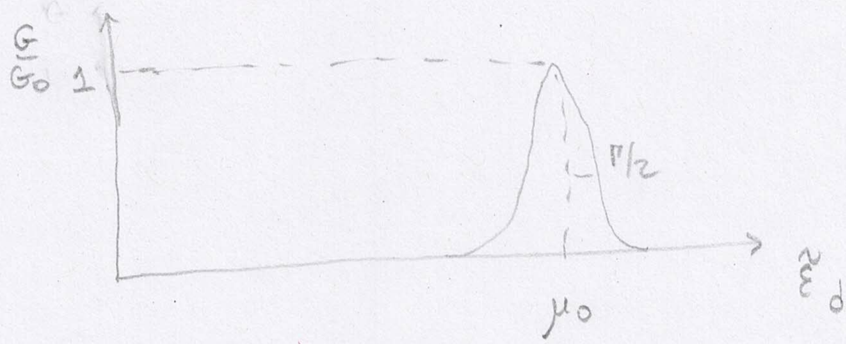
$\frac{G}{G_0} \rightarrow \frac{2}{3}$ for large $\frac{U}{\Gamma}$

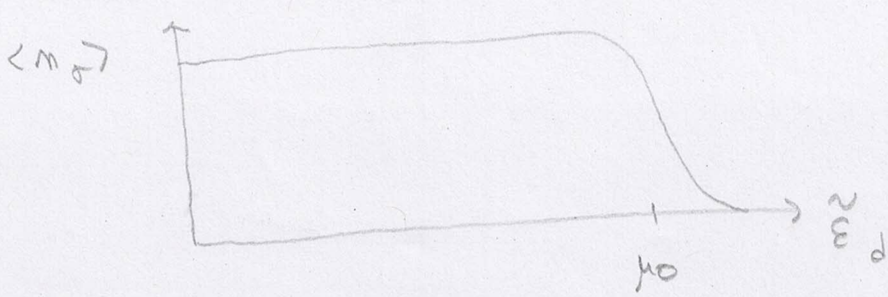
Here, however, our approx breaks!



on the other hand

$U = 0$





2nd limiting case for the conductance: $\Gamma \to 0$

$\boxed{\Gamma \to 0} \Rightarrow \Gamma \ll T, U$ $\qquad$ Γ is the smallest energy scale

Let us turn back to the conductance expression

$$G = e^2 \sum_\sigma \int \frac{d\varepsilon}{2\pi} \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} A_\sigma(\varepsilon/\hbar) \left(-\frac{\partial f}{\partial \varepsilon}\right)$$

we have now two competing broadenings,

one from $A_\sigma(\varepsilon/\hbar) \Rightarrow \Gamma$

one from $\left(\frac{-\partial f}{\partial \varepsilon}\right) \Rightarrow k_B T$

Since $k_B T \gg \Gamma$, the spectral function $A_\sigma(\varepsilon/\hbar)$ behaves like a very sharply peaked function.

Use

$$\lim_{\Gamma \to 0} \frac{\hbar\Gamma/2}{(\hbar\omega - \varepsilon_i)^2 + (\hbar\Gamma/2)^2} = \pi\,\delta(\hbar\omega - \varepsilon)$$

$\delta_\varepsilon(x) = \frac{1}{\pi} \frac{\varepsilon}{x^2 + \varepsilon^2}$.

like for the non-interacting case

$$\boxed{G = e^2 \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} \sum_\sigma \left[\left(-\frac{\partial f}{\partial \varepsilon}\right)\Big|_{\varepsilon = \tilde{\varepsilon}_\sigma} (1 - \langle \hat{n}_{\bar{\sigma}} \rangle) + \left(-\frac{\partial f}{\partial \varepsilon}\right)\Big|_{\varepsilon = \tilde{\varepsilon}_\sigma + U} \langle \hat{n}_{\bar{\sigma}} \rangle\right]}$$

(4.113)

further, from (4.108) where $\langle \hat{n}_\sigma \rangle = \langle \hat{n}_{\bar{\sigma}} \rangle = \frac{n_o}{1 + n_o - n_u}$

$$\hookrightarrow \boxed{\langle \hat{n}_\sigma \rangle = \frac{f(\tilde{\varepsilon}_d)}{1 + f(\tilde{\varepsilon}_d) - f(\tilde{\varepsilon}_d + U)}} \quad (4.114)$$

Hence if $\varepsilon_\sigma = \varepsilon_{\bar\sigma} = \tilde\varepsilon_d$ and using

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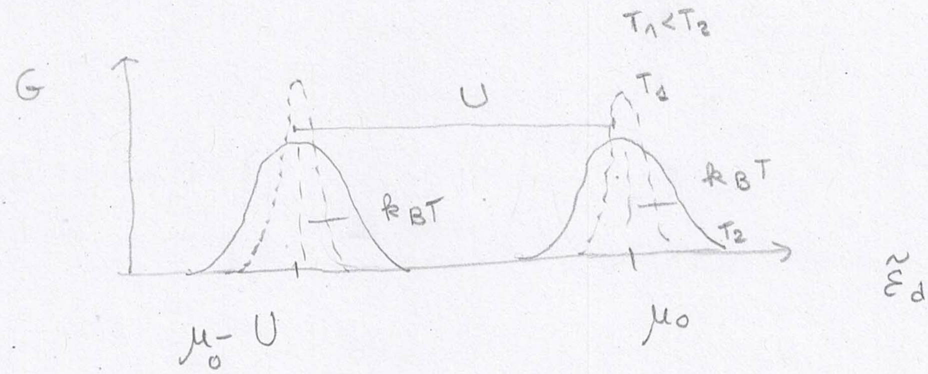
$$-\frac{\partial f}{\partial \varepsilon} \underset{(*)}{=} \frac{1}{4k_BT}\,\frac{1}{ch^2\,\beta\frac{(\varepsilon-\mu_0)}{2}} \qquad (4.115)$$

it follows, for $\Gamma_L = \Gamma_R = \frac{\Gamma}{2}$ $\left(\Rightarrow \frac{\Gamma_L\Gamma_R}{\Gamma_L+\Gamma_R} = \frac{\Gamma}{4}\right)$

$$\boxed{G = 2e^2\frac{\Gamma}{4}\frac{1}{4k_BT}\left[\frac{1}{ch^2\,\beta\frac{(\tilde\varepsilon_d-\mu_0)}{2}}\,\frac{1-f(\tilde\varepsilon_d+U)}{1+f(\tilde\varepsilon_d)-f(\tilde\varepsilon_d+U)} + \frac{1}{ch^2\,\beta\frac{(\tilde\varepsilon_d+U-\mu_0)}{2}}\,\frac{f(\tilde\varepsilon_d)}{1+f(\tilde\varepsilon_d)-f(\tilde\varepsilon_d+U)}\right]} \qquad (4.116)$$



$G \ll G_0$

$\Rightarrow$ i) conductance peaks increase as $\sim \frac{1}{T}$ when T is lowered
ii) broadening is $\sim k_BT$

(*) $f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu_0)}+1}$, $\frac{\partial f}{\partial \varepsilon} = -\left(e^{\beta(\varepsilon-\mu_0)}+1\right)^{-2}\beta\, e^{\beta(\varepsilon-\mu_0)}$

$$= -\frac{1}{k_BT}\frac{e^{\beta(\varepsilon-\mu_0)}}{(1+e^{\beta(\varepsilon-\mu_0)})^2} = -\frac{1}{k_BT}\frac{1}{\left(e^{\beta(\varepsilon-\mu_0)/2}+e^{-\beta(\varepsilon-\mu_0)/2}\right)^2} =$$