KELDYSH STRUCTURE OF VERTICES

REMEMBER: SINGLE-PARTICLE POT.

P_1, P_2 OTHER DEGR. OF FREEDOM

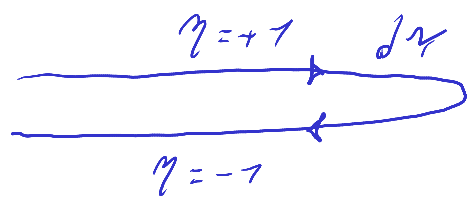
$$\int G(\cdots|\gamma_1 P_1)\, V(\gamma_1 P_1, \gamma_2 P_2)\, G(\gamma_2 P_2|\cdots)$$

$$\Rightarrow V(\gamma_1 P_1, \gamma_2 P_2) = \delta(\gamma_1 - \gamma_2)\, V(P_1, P_2, t_1)$$

$$\gamma_1 = \gamma_2 \doteq \gamma = (t, \eta)$$

$$= \int d\gamma\, G(\cdots|\gamma P_1)\, V(P_1, P_2, t)\, G(\gamma P_2|\cdots)$$

$$\int d\gamma \doteq \sum_\eta \int dt \cdot \eta$$



(CF. A22, A23)

$$= \int dt\, \hat{G}(\cdots|tP_1)\, \underbrace{\gamma_3\, V(P_1, P_2, t)}_{\hat{V}(P_1, P_2, t)}\, \hat{G}(t, P_2|\cdots)$$

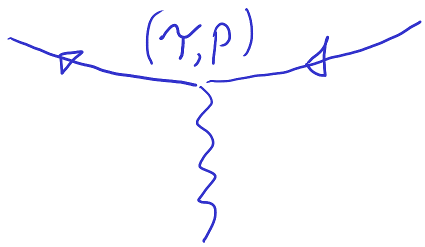
(cf. A24,A242, A26)

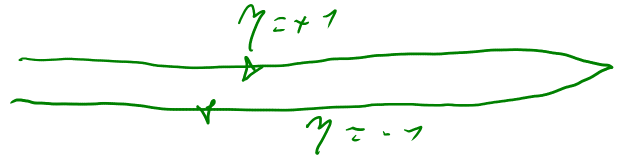
$$\doteq \int dt\, \underline{G}(\cdots|tP_1)\, \underbrace{I\, V(P_1, P_2, t)}_{\underline{V}(P_1, P_2, t)}\, \underline{G}(tP_2|\cdots) \qquad \text{(D1)}$$

Electron-phonon and electron-electron vertices

EL. - PHONON

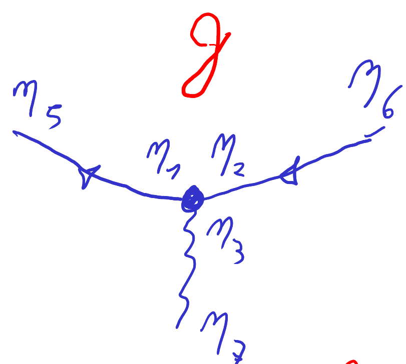
$$\gamma = (\eta, t)$$





(OMIT OTHER DEG. OF FR. p_i)

$$\int d\gamma = \sum_\eta \int dt \cdot \eta$$



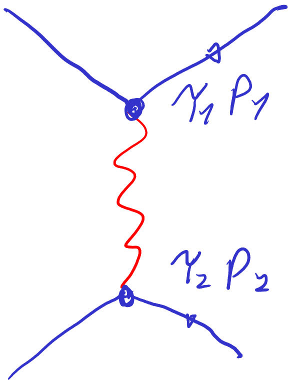
PHONON GREEN'S FUNCTION

$$g(\ldots)\,\underbrace{\eta_1\,\delta_{\eta_1\eta_2}\,\delta_{\eta_1\eta_3}}_{\hat{\gamma}^{\eta_3}_{\eta_1\eta_2}}\,\hat{G}_{\eta_5\eta_1}\,\hat{G}_{\eta_2\eta_6}\,\hat{D}_{\eta_3\eta_7} \qquad \text{(D2)}$$

(convention: A22)

SAME INDEX STRUCTURE FOR EL.-EL. INTERACTION

EL.-PH.

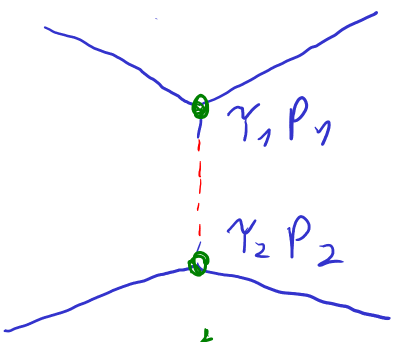


$\gamma_1 P_1 = \eta_1 t_1 P_1$

$\gamma_2 P_2 = \eta_2 t_2 P_2$

$$\Rightarrow g(\dots)\, g(\dots)\, D(t_1 P_1, t_2 P_2)_{\eta_1, \eta_2}$$

EL.-EL.



$\gamma_1 P_1$

$\gamma_2 P_2$

$g = 1$

Formally $g(\dots) \longrightarrow 1$

$$D(t_1 P_1, t_2 P_2)_{\eta_1, \eta_2} \longrightarrow U(P_1 P_2, t_1)\, \delta_{\eta_1 \eta_2}\, \delta(t_1 - t_2)$$

→ TRANSFORMING $\hat{G}, \hat{D}$ INTO $\underline{G}$ $\underline{D}$

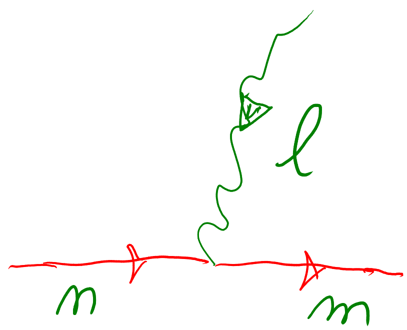
(cf. A24)

(SEE RAMMER-SMITH 1986)

IT IS CONVENIENT TO DISTINGUISH: ABSORPTION, EMISSION

WE USE INDICES $n, m, \ell = 1, 2$

Phonon absorption:



$$= \frac{g}{\sqrt{2}} \gamma_{n,m,\ell} \tag{D3}$$

(proof in DET1)

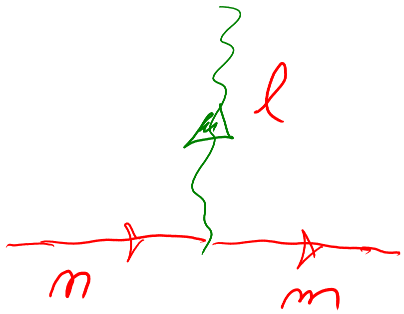
g IS THE AMPLITUDE, WHICH DEPENDS ON OTHER DEGREES OF FREEDOM

$$\gamma_{n,m,\ell} = \delta_{\ell,1} \delta_{n,m} + \delta_{\ell,2} \tau^{1}_{n,m}$$

or in other words

$$= \begin{cases} 1 & \text{if an even number of the indices } n,m,l \text{ is } 2 \\ 0 & \text{otherwise} \end{cases} \tag{D4}$$

Phonon emission:



$$= \frac{g}{\sqrt{2}} \tilde{\gamma}_{n,m,l} \qquad \text{(D5)}$$

with

$$\tilde{\gamma}_{n,m,l} = \gamma_{n,m,\bar{l}} = 1 - \gamma_{nml}$$

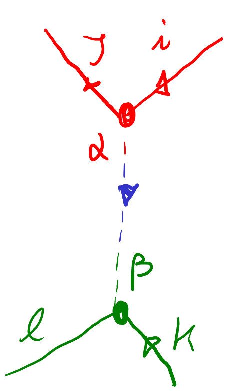
$$\bar{l} = \begin{cases} 1 & l = 2 \\ 2 & l = 1 \end{cases} \qquad \text{(D6)}$$

(proof in DET1)

The same shape is for the elctron-electron interaction vertex

Notice that here emission or absorption cannot be distinguished, but one can fix arbitrarily a direction for each line: it does not matter.

SUM CONVENTION



$$U_{El.-El.} = U(\dots) \frac{\tilde{\gamma}_{ij\alpha}}{\sqrt{2}} \frac{\gamma_{kl\beta}}{\sqrt{2}} \delta_{\alpha\beta}$$

$$= \frac{1}{2} U(\dots) \tilde{\gamma}_{ij\alpha} \gamma_{kl\alpha} = \frac{1}{2} U(\dots) \gamma_{ij\bar{\alpha}} \gamma_{kl\alpha}$$

$$\gamma_{kl\alpha}: \quad \alpha = 2 \Rightarrow k \neq l \qquad \alpha = 1 \Rightarrow k = l$$

(cf. D4, D6)

$$\gamma_{ij\bar{\alpha}}: \quad \alpha = 2 \Rightarrow i = j \qquad \alpha = 1 \Rightarrow i \neq j$$

$$U_{El.-El.} = \frac{U(\dots)}{2} \sum_{\alpha} \gamma_{kl\alpha}\, \gamma_{ij\bar{\alpha}} = \frac{U(\dots)}{2} \left(\delta_{k=l}\, \delta_{i \neq j} + \delta_{k \neq l}\, \delta_{i=j} \right) \tag{D7}$$

Application

Hartree diagram

EQUAL TIMES:

Whenever one encounters in a diagram a time-ordered Greens function where the time arguments are equal, one takes the average over the two orderings:
EXAMPLE:

= time ordered

$$G^c(t_1,t_1) = -i\langle T\,\psi(t_1)\,\psi^+(t_1)\rangle$$

$$= -\frac{i}{2}\langle \psi(t_1)\psi^+(t_1) - \psi^+(t_1)\psi(t_1)\rangle =$$

$$= i\langle \psi^+(t_1)\psi(t_1) - \frac{1}{2}\rangle$$

This is in contrast to equilibrium theory, whereby the convention is that the second time acquires a positive infinitesimum

$$G^c(t_1, t_1+0^+) = i\langle \psi^+(t_1)\psi(t_1)\rangle$$

If we wanted that the "dag" always stays on the left at equal times, then the infinitesimum should be negative in the second (backward) time branch. In this way, we could not write a single Keldys Green's function matrix.

This convention is allowed provided we assume that the Hamiltonian is understood to be written not in normal ordering (as one does in equilibrium) but in symmetric ordering, e.g

$$\psi^+(x)\,\psi(x) \rightarrow \,:\psi^+(x)\,\psi(x): \,\equiv \frac{1}{2}\left(\psi^+(x)\,\psi(x) - \psi(x)\,\psi^+(x)\right)$$

(here for fermions)

E.g. the Hubbard interaction

$$U \underbrace{\psi^\dagger_\uparrow \psi_\uparrow}_{\hat{n}_\uparrow} \underbrace{\psi^\dagger_\downarrow \psi_\downarrow}_{\hat{n}_\downarrow} = U \hat{n}_\uparrow \hat{n}_\downarrow$$

$$= U\left(:\hat{n}_\uparrow: + \frac{1}{2}\right)\left(:\hat{n}_\downarrow: + \frac{1}{2}\right) =$$

$$= U\left(:\hat{n}_\uparrow \hat{n}_\downarrow: + \frac{1}{2}\left(:\hat{n}_\uparrow + \hat{n}_\downarrow:\right) + \frac{1}{4}\right)$$

which changes the on-site energy term

A consequence of this assumed ordering: there are never convergence factors, and integrals over frequency can be symmetrized even when the integrand falls off as $1/\omega$

In other words: one takes the Cauchy principal value at infinity

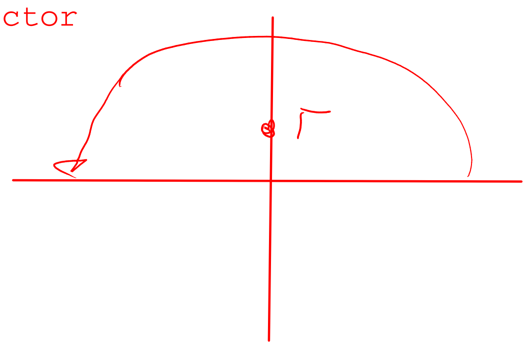
e.g.

$$P\int \frac{d\omega}{2\pi} \frac{1}{\omega + i\Gamma} = \int \frac{d\omega}{2\pi} \frac{1}{2}\left(\frac{1}{\omega + i\Gamma} + \frac{1}{-\omega + i\Gamma}\right) = -i \int \frac{d\omega}{2\pi} \frac{\Gamma}{\Gamma^2 + \omega^2}$$

$$= -\frac{i}{2} \operatorname{sgn} \Gamma$$

This is different if one has a convergence factor

$$\int \frac{d\omega}{2\pi} \frac{1}{\omega + i\Gamma} e^{i0^+\omega} = i\,\Theta(-\Gamma)$$

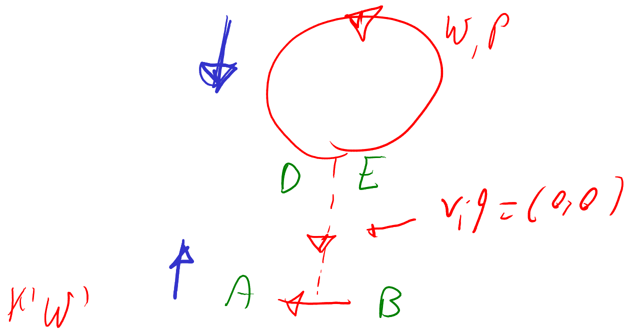


The two differ again by a i/2

Let us now illustrate this by evaluating the Hartree diagram

We take for simplicity the Hubbard model with $\hat{U}_{El.-El.} = \sum_R U :\hat{n}_{R\uparrow}\hat{n}_{R\downarrow}:$

(D9)



D, E A, B

KELDYSH INDICES

(cf. D7)

$$\propto \frac{U}{2}\left(\delta_{A=B}\,\delta_{D\neq E} + \delta_{A\neq B}\,\delta_{D=E}\right)$$

(D10)

contribution to retarded self-energy A=B=1

$$\longrightarrow \quad D=1 \quad E=2 \quad \Rightarrow G^0_K$$
$$D=2 \quad E=1 \quad \Rightarrow 0$$

fermion loop

$$-\frac{i}{2}\,U(q=0)\int\frac{d\omega}{2\pi}\,\frac{1}{V}\sum_{\vec{p}} G^0_K(\vec{p},\omega,t)$$

for the Hubbard model $U(q=0) = U$

(CF B-1)

$$= U\,\frac{1}{V}\sum_{p}\left(n_{p\downarrow} - \frac{1}{2}\right) = U\left(n_{R\downarrow} - \frac{1}{2}\right)$$

$$= U\left\langle :\hat{n}_{R\downarrow}:\right\rangle$$

particle density with one spin

(D11)

The Hartree contribution comes from a decoupling of the interaction term

To obtain the result above we have to assume that the interaction term is

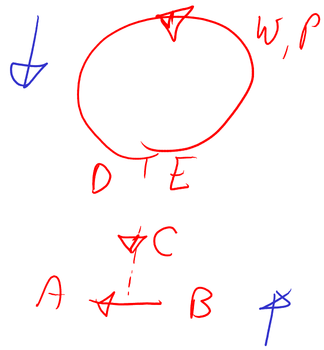
$$\hat{U}_{El.-El.} = \sum_R U :\hat{n}_{R\uparrow}\hat{n}_{R\downarrow}:$$

which in mean-field decouples to

$$\sum_R \Big(U \langle :\hat{n}_{R\downarrow}: \rangle :\hat{n}_{R\uparrow}: + U \langle :\hat{n}_{R\uparrow}: \rangle :\hat{n}_{R\downarrow}: \Big) + \text{const.}$$

giving the correct energy shift $U \langle :\hat{n}_{R\downarrow}: \rangle$

We evaluate the contribution to the Keldysh self-energy $A=1 \quad B=2 \quad \to \quad D=E=1,2$



$$\propto \frac{1}{V}\sum_p \int \frac{d\omega}{2\pi}\left(G^0_r(p,\omega)+G^0_a(p,\omega)\right)$$

$$G^0_r + G^0_a \propto \frac{1}{\omega-\epsilon_p+i\delta}+\frac{1}{\omega-\epsilon_p-i\delta}$$

$$= \frac{2(\omega-\epsilon_p)}{(\omega-\epsilon_p)^2+\delta^2}$$

This is odd in $\omega-\epsilon_p$

and thus its integral over $d\omega$ vanishes

$\int d\omega$

The contribution is 0

$$\int \frac{\omega}{\omega^2+T^2}\, e^{i\omega 0^+}\, d\omega \neq 0$$

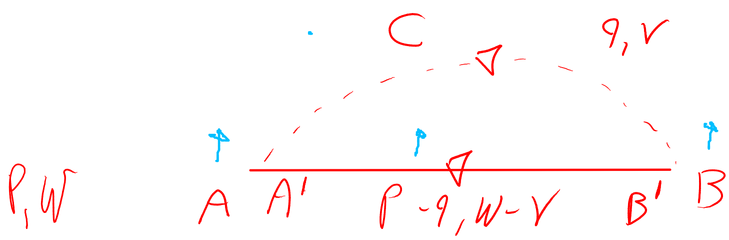
Fock diagram   Notice that for Hubbard model this is in fact zero

WE CONSIDER GENERIC TERM:

$$\hat{U}_{EL-EL} = \frac{1}{2} \sum_{\substack{R,R' \\ \sigma,\sigma'}} V(R-R')\, C^{+}_{R,\sigma} C_{R,\sigma} C^{+}_{R'\sigma'} C_{R'\sigma'} =$$

$$\frac{1}{2}\frac{1}{V} \sum_{\substack{p\,p' \\ q,\sigma,\sigma'}} V(q)\, C^{+}_{p,\sigma} C^{+}_{p',\sigma'} C_{p'-q,\sigma'} C_{p+q,\sigma} \qquad \text{(D12)}$$

(: :) TO KEEP IN MIND



1) Σ_r : $A=B=1$

(CF D7) $\frac{V(q)}{2}\left(\delta_{AA'}\,\delta_{B\neq B'} + \delta_{A\neq A'}\,\delta_{B=B'}\right)$

$A=B=1 \quad = \underbrace{\delta_{1A'}\,\delta_{B'2} + \delta_{A'2}\,\delta_{B'1}}_{G_K}$

$$\Sigma_r(p,\omega) = \frac{i}{2}\int d_4 q\; V(\vec{q})\; G^{0}_{K}(p-q,\omega-\nu)$$

$$= \frac{i}{2}\,\frac{1}{V}\sum_q V(\vec{q})\,\frac{d\nu}{\cancel{2\pi}}\,(-\cancel{2}i\pi)\,\overbrace{\underbrace{A_0(p-q,\omega-\nu)}_{\delta(\omega-\nu-\varepsilon_{p-q})}\, S(\omega-\nu)}^{\text{EQUIL.}} \qquad \text{(D13)}$$

$$= \frac{1}{2}\,\frac{1}{V}\sum_q V(\vec{q})\; S(\varepsilon_{p-q})$$

real, ω independent: just an energy shift

SELF-CONSISTENT:

WE ASSUME STEADY STATE (TIME TRANSL.)

D13 becomes instead:

$$\Sigma_n(p,w) = \frac{i}{2}\frac{1}{V}\sum_q V(q)\underbrace{\int\frac{d\nu}{2\pi}G_K(p-q,w-\nu)}_{G_K(p-q,t=0)}$$

(CF. B-1) $= 2i\langle c^\dagger_{p-q}c_{p-q}\rangle - i\,\delta_{p-q,0}$

SAME SPIN

$$= -\frac{1}{V}\sum_{p'}\langle c^\dagger_{p'\uparrow}c_{p'\uparrow}\rangle V(p-q') \qquad \text{(D14)}$$

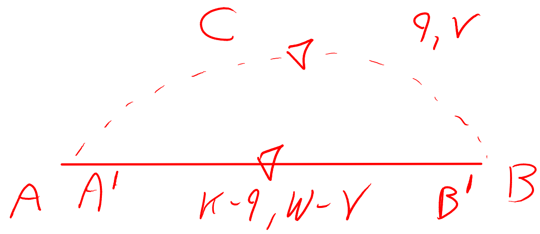
AGAIN THIS COMES FROM A DECOUPLING OF THE INTERACTION TERM (cf. D12)

$$\hat{U}_{EL-EL} = \frac{1}{2}\frac{1}{V}\sum_{\substack{p\,p'\\ q,\sigma,\sigma'}} V(q)\,c^\dagger_{p,\sigma}\underbrace{c^\dagger_{p',\sigma'}c_{p'-q,\sigma'}}c_{p+q,\sigma}$$

$$\Rightarrow -\frac{1}{V}\sum_{\substack{p,p'\\ q,\sigma,\sigma'}} V(q)\langle \underbrace{c^\dagger_{p'\sigma'}c_{p+q\sigma}}_{\substack{p+q=p' \Rightarrow q=p'-p\\ \sigma=\sigma'}}\rangle c^\dagger_{p,\sigma}c_{p'-q,\sigma'}$$

$$= \underbrace{-\frac{1}{V}\sum_{\substack{p,p'\\ \sigma}} V(p'-p)\langle c^\dagger_{p'\sigma}c_{p'\sigma}\rangle}_{\Sigma_n(p,w)} c^\dagger_{p\sigma}c_{p\sigma}$$

keldysh contribution



$A=1 \quad B=2 \quad \Rightarrow \quad A'=B'$ (cf. D7)

$$\Sigma_k \propto \int d\nu \left(g_r(\omega-\nu) + g_a(\omega-\nu) \right) = 0$$

SHIFT $\omega - \nu \to \nu$

$$g_r(\nu) + g_a(\nu) = \frac{1}{\nu - \varepsilon_k + i\delta} + \frac{1}{\nu - \varepsilon_k - i\delta}$$

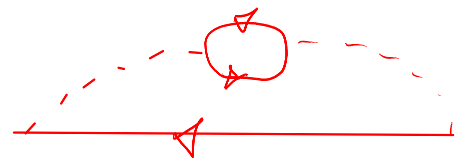
$$= \frac{\nu - \varepsilon_k}{(\nu-\varepsilon_k)^2 + \delta^2}$$

odd in $\nu - \varepsilon_k$

$\to$ INTEGRAL 0

Hartree and Fock terms only produce a shift of the energy

First notrivial diagram:



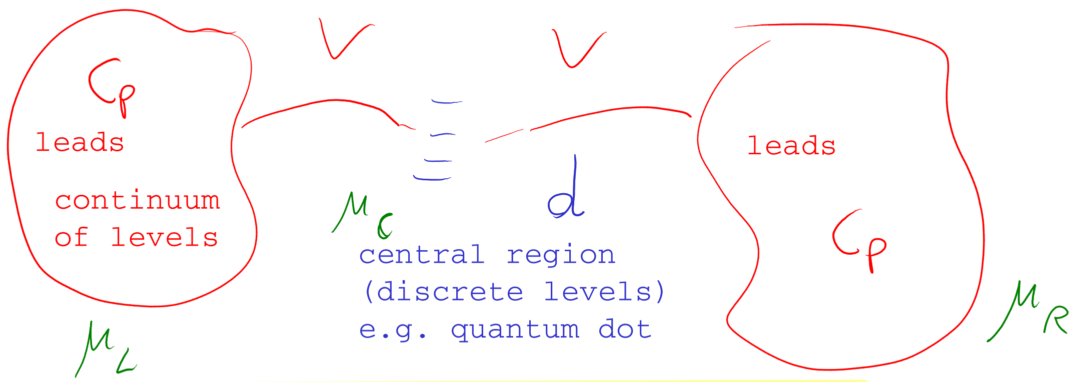
but we are not going to evaluate it like this

Transport through mesoscopic structures effects of electron-electron interaction

"Hubbard I" or "cluster perturbation theory" approximations

(see Haug-Jauho's Book)

Single Impurity Anderson model



Electron-electron interaction U
in central region

For simplicity, we study again the case of
a single level. Extension to many levels
is, in principle straightforward

$$H_0 = \underbrace{\sum_{p,s} \varepsilon_p c^\dagger_{ps} c_{ps}}_{\text{leads}} + \underbrace{\overbrace{\left(\Delta - \frac{U}{2}\right)}^{\varepsilon_d} \sum_s d_s^\dagger d_s}_{\text{central region}}$$

$$V = \underbrace{\sum_{p,s} V_p \left(c^\dagger_{ps} d_s + d_s^\dagger c_{ps} \right)}_{\text{coupling}}$$

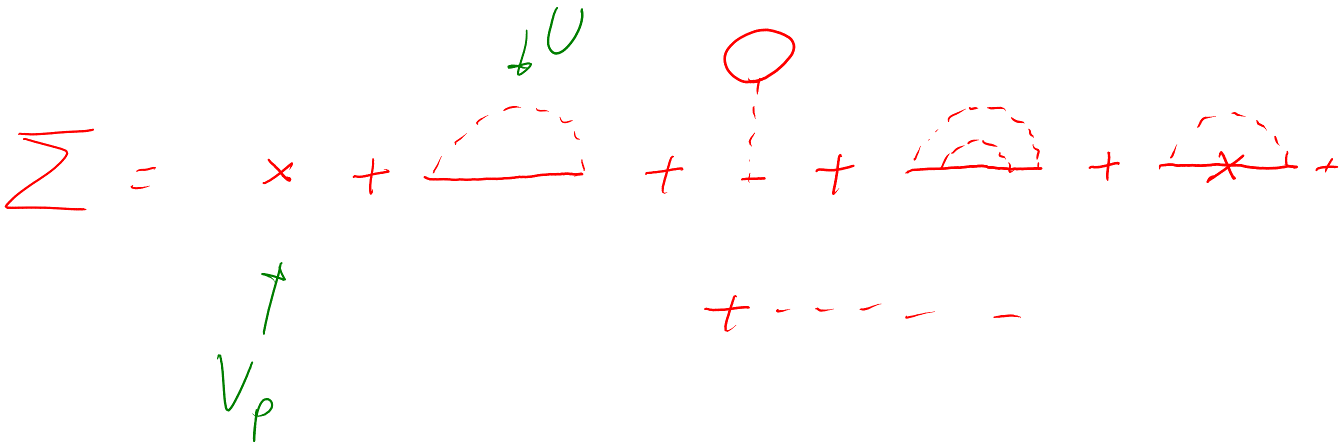
$$+ U d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow \qquad \text{(D15)}$$

here again one dot level only

PRODUCES: (1) COULOMB BLOCKADE (2) KONDO EFFECT

Self energy:

In principle one can have for example these diagrams:



However there are two properties

1) U attaches to d sites ony

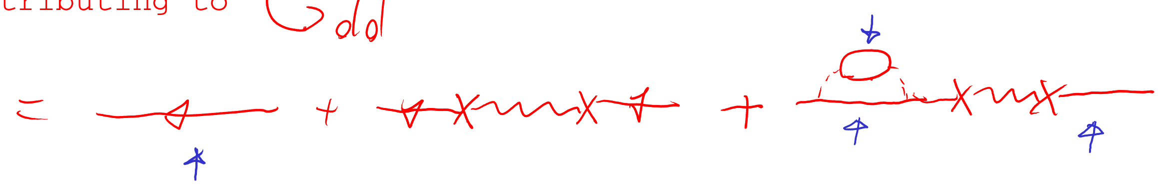
2) Vp only connects c with d

It is convenient, thus, to distinguish c and d Green's functions

g_{dd}

g_{cc}

Some diagrams contributing to G_{dd}



Now consider the d-d self energy $\tilde{\Sigma}$ which is the sum of diagrams that cannot be taken apart by breaking a d-line (i.e. )

It gives the Dyson equation

$$G_{dd} = g_{dd} + g_{dd}\,\tilde{\Sigma}\,G_{dd}$$

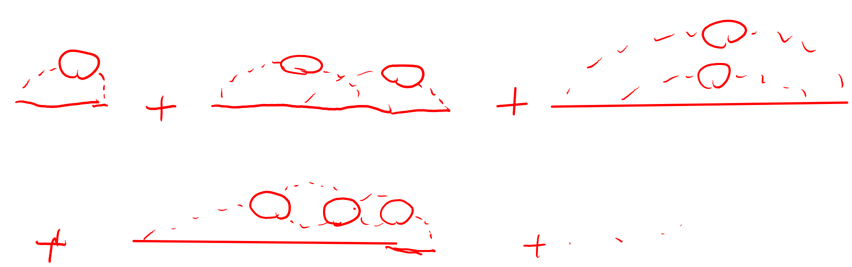
$\tilde{\Sigma} =$ 

notice that for $U=0$ only the first diagram contributes

and we recover the result that we already know

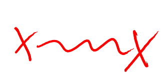
$\tilde{\Sigma}(U=0) = V_{0p}\,g_{pp}\,V_{p0} =$ 

We can consider the sum of all diagrams not containing any V

$\tilde{\Sigma}(V=0) =$ 

this can be evaluated exactly since it is the exact solution of the single-site model (or a small cluster)

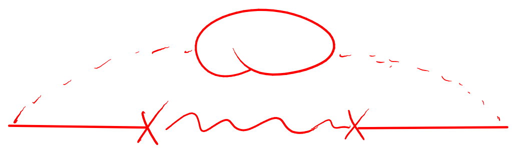
Then one can take as an approximation

$\tilde{\Sigma} = \tilde{\Sigma}(V=0) +$  $= \tilde{\Sigma}(V=0) + \tilde{\Sigma}(U=0)$

This is the "Hubbard I" approximation

Extensions: take a central region consisting of many levels:
Cluster Perturbation Theory (cf. Balzer-Potthoff 2011)

The first neglected diagram contains both V and U:



WE NEED THE SINGLE SITE
SELF ENERGY

FIRST WE EVALUATE THE GREEN'S FCT.

ONE COULD USE EXACT DIAGONALIZATION
(ALSO FOR A SMALL CLUSTER)
AND LEHMAN'S REPRESENTATION

HERE, WE WILL USE THE EQUATIONS OF MOTION
$G^{RET}_{dd}(V=0)$ (INDICES OMITTED FOR SIMPLICITY)

$$\mathcal{G}(t) = -i\,\Theta(t)\langle\{d_\uparrow(t), d_\uparrow^\dagger(0)\}\rangle$$

$$i\partial_t \mathcal{G} = \delta(t)\cdot 1 + \Theta(t)\langle\{\partial_t d_\uparrow(t), d_\uparrow^\dagger(0)\}\rangle$$

$$H = \varepsilon_d \sum_\sigma d_\sigma^\dagger d_\sigma + U n_\uparrow n_\downarrow$$

$$\partial_t d_\uparrow(t) = i[H, d_\uparrow(t)] = i(-\varepsilon_d d_\uparrow - U n_\downarrow d_\uparrow) \tag{D16}$$

$$i\partial_t \mathcal{G} = \delta(t) - i\Theta(t)\left(\varepsilon_d\langle\{d_\uparrow(t), d_\uparrow^\dagger\}\rangle + U\langle\{n_\downarrow(t)d_\uparrow(t), d_\uparrow^\dagger\}\rangle\right)$$

$$= \delta(t) + \varepsilon_d\,\mathcal{G}(t) + U\mathcal{G}^{(2)}(t) \tag{D17}$$

FOURIER TRANSFORM $\int_{-\infty}^{+\infty} e^{i(W+i0^+)}$

AND PARTIAL INTEGRATION GIVES

$$W\, g(W) = 1 + \varepsilon_d\, g(W) + U\, g^{(2)}(W) \qquad (W \to W + i0^+)$$

WE NEED $g^{(2)}(t) = -i\,\Theta(t)\langle\{n_\downarrow d_\uparrow(t), d_\uparrow^\dagger\}\rangle$

$$[H, n_\downarrow(t)] = 0 \implies n_\downarrow \text{ INDEP. OF } t$$

FOR $t=0$ $\langle\{\ldots\}\rangle = \langle n_\downarrow \{d_\uparrow, d_\uparrow^\dagger\}\rangle = \langle n_\downarrow\rangle$

$$i\,\partial_t\, g^{(2)}(t) = \delta(t)\langle n_\downarrow\rangle + \Theta(t)\langle\{n_\downarrow\, \partial_t d_\uparrow(t), d_\uparrow^\dagger\}\rangle$$

(see D16) AND USING $n_\downarrow^2 = n_\downarrow$ (FERMIONS)

$$= \delta(t)\langle n_\downarrow\rangle - i\,\Theta(t)\,(\varepsilon_d + U)\langle\{n_\downarrow d_\uparrow(t), d_\uparrow^\dagger\}\rangle$$

$$= \delta(t)\langle n_\downarrow\rangle + (\varepsilon_d + U)\, g^{(2)}(t)$$

$$\implies \quad W\, g^{(2)}(W) = \langle n_\downarrow\rangle + (\varepsilon_d + U)\, g^{(2)}(W)$$

$$\implies \quad g^{(2)}(W) = \frac{\langle n_\downarrow\rangle}{(W - \varepsilon_d - U)} \qquad \text{(D18)}$$

$$\Rightarrow \quad (w-\varepsilon)\, g(w) = 1 + U g^{(2)}(w)$$

$$g = \frac{1 + U \dfrac{\langle n_\downarrow \rangle}{w - \varepsilon_d - U}}{w - \varepsilon} = \frac{\langle n_\downarrow \rangle}{w - \varepsilon_d - U} + \frac{1 - \langle n_\downarrow \rangle}{w - \varepsilon_d}$$

TWO POLES $w = \varepsilon + U \quad \propto \langle n_\downarrow \rangle$

$w = \varepsilon \quad \propto 1 - \langle n_\downarrow \rangle$

(cf. D15)

$$g = \frac{\langle n_\downarrow \rangle}{w - \Delta - \frac{U}{2}} + \frac{1 - \langle n_\downarrow \rangle}{w - \Delta + \frac{U}{2}} = G^R(V=0)$$ (D19)

FOR $w \to w + i0^+$ IT'S g_R FOR $w \to w - i0^+$ IT'S g_A

g_K CAN BE OBTAINED BY

$$g_K = (g_R - g_A)\, s(w)$$ (cf. A7)

WE NEED THE INVERSE (SELF-ENERGY)

$$(g^{-1})_R = (g_R)^{-1}$$ (cf. A9)

$$(g^{-1})_K = -g_R^{-1}\, g_K\, g_A^{-1} = (g_R^{-1} - g_A^{-1})\, s(w)$$

BUT $g_R^{-1} - g_A^{-1}$ IS NONZERO ONLY NEAR THE POLES OF g_R

$\Rightarrow \quad g_R^{-1} - g_A^{-1} \propto 0^+$ INFINITESIMAL

$\Rightarrow \Sigma_K$ CAN BE NEGLECTED AS IN NONINTERACTING CASE

COUPLING TO THE LEADS

THE SELF-ENERGY CAN BE EXTRACTED BY

$$g_{dd}^{-1} - \tilde{\Sigma}(V=0) = G(V=0)^{-1}$$

Within this "Hubbard I" approximation, we obtain (cf. D15A)

$$G_{dd} = \left(g_{dd}^{-1} - \tilde{\Sigma}(V=0) - \tilde{\Sigma}(U=0) \right)^{-1}$$

$$= \left(\underbrace{G(V=0)^{-1}}_{\text{THIS WE JUST CALCULATED}} - \sum_p V_{0p}\, g_{pp}\, V_{p0} \right)^{-1} \qquad \text{(D19A)}$$

THESE ARE 2x2 KELDYS MATRICES

THE RETARDED PART AS USUAL (cf. A9)

$$G_{dd}^{R} = \left(G^{R}(V=0)^{-1} - \sum_p V_{0p}^{2}\, g_{pp} \right)^{-1} = \left(G^{R}(V=0)^{-1} - R(\omega) + i\,\Gamma(\omega) \right)^{-1} \qquad \text{(D20)}$$

AS FOR THE NONINTERACTING CASE, WE HAVE TAKEN V_{0p} = CONST.

SO THAT $\sum_p g_{pp}^{R} = R(\omega) - i\,\Gamma(\omega)/V^{2}$ (cf. B6A, B6B)

Using D19,D20, AND ASSUMING R, Γ WEAKLY ω-DEPENDENT

$$G^R_{dd} = \left(\left(\frac{\langle n_\downarrow \rangle}{\omega - \Delta - \frac{U}{2}} + \frac{1 - \langle n_\downarrow \rangle}{\omega - \Delta + \frac{U}{2}} \right)^{-1} - R + i\Gamma \right)^{-1}$$

THE TERM IN $(\cdots)$ IS DOMINATED BY THE POLES AT $\omega = \Delta \pm \frac{U}{2}$

FOR $R, \Gamma \ll U$ WE CAN JUST LOOK NEAR THESE POLES

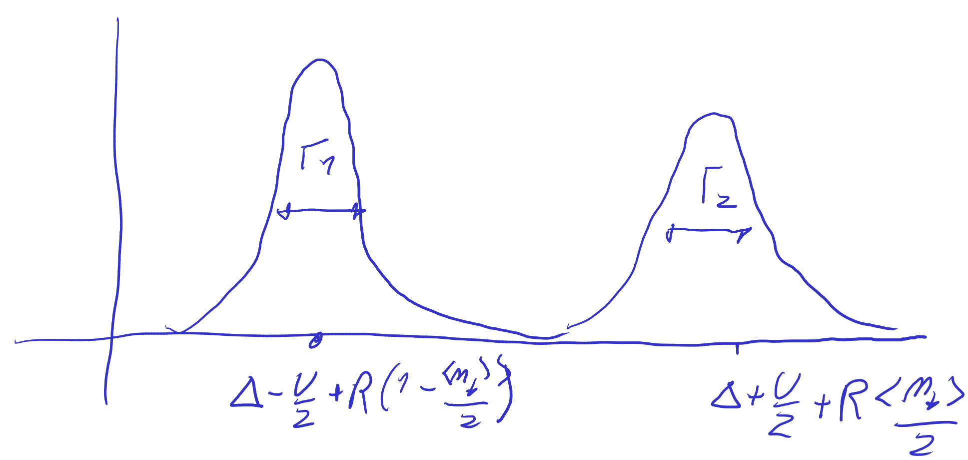
E.G. FOR $\omega \sim \Delta + \frac{U}{2}$

$$G^R_{dd} \approx \left(\frac{\omega - \Delta - \frac{U}{2} - R\langle n_\downarrow \rangle + i\Gamma \langle n_\downarrow \rangle}{\langle n_\downarrow \rangle} \right)^{-1}$$

SO THE POLE IS SHIFTED AND BROADENED

THE CORRSPONDING SPECTRAL FUNCTION:

$$A_{dd} = -\frac{1}{\pi} \operatorname{Im} G^R_{dd} =$$



THE CALCULATION OF THE CURRENT IS SIMILAR TO THE NONINTERACTING CASE

1) EVALUATE G^{K}_{dd}

THIS REQUIRES Σ^{K}. SINCE THE CONTRIB. FROM THE DOT IS INFINITESIMAL ONLY THE LEADS CONTRIBUTED SO ONE ENDS UP WITH AN EXPR. SIMILAR TO (B6)

$$G^{K}_{dd} = -2i\pi V^{2} \left| G^{r}_{dd}(\omega) \right|^{2} \left(\rho^{0}_{L}(\omega)\, h_{L}(\omega) + \rho^{0}_{R}(\omega)\, h_{R}(\omega) \right)$$

$$= \left(G^{r}_{dd}(\omega) - G^{a}_{dd}(\omega) \right) h_{AV}(\omega)$$

$$h_{AV}(\omega) \equiv \frac{\rho^{0}_{L}(\omega)\, h_{L}(\omega) + \rho^{0}_{R}(\omega)\, h_{R}(\omega)}{\rho^{0}_{L}(\omega) + \rho^{0}_{R}(\omega)}$$

This can be used to evaluate the particle density $\langle n \rangle$

Also the rest of the discussion is similar

$$I = e V^2 \int dw \; \gamma(w)$$

$$\gamma(w) = 2\pi \; A_{dd}(w) \; \frac{\rho_L^0 \rho_R^0}{\rho_L^0 + \rho_R^0} \left(f_F(w-\mu_L) - f_F(w-\mu_R) \right)$$

equivalently

$$\gamma(w) = 2\pi V^2 \left| G_{dd}^r \right|^2 \rho_L^0 \rho_R^0 \left(f_F(w-\mu_L) - f_F(w-\mu_R) \right)$$

Taking 0 temperature and $\mu_R < \mu_L$

$$I = 2\pi \; e V^2 \int_{\mu_R}^{\mu_L} dw \; A_{dd}(w) \; \frac{\rho_L^0 \rho_R^0}{\rho_L^0 + \rho_R^0} \tag{D21}$$

THE EFFECT OF THE INTERACTION IS ONLY IN G_{dd}^r (OR, EQUIVALENTLY A_{dd})

From the expression for the current

$$I \propto \int_{\mu_R}^{\mu_L} A_{dd}(\omega)\, d\omega$$

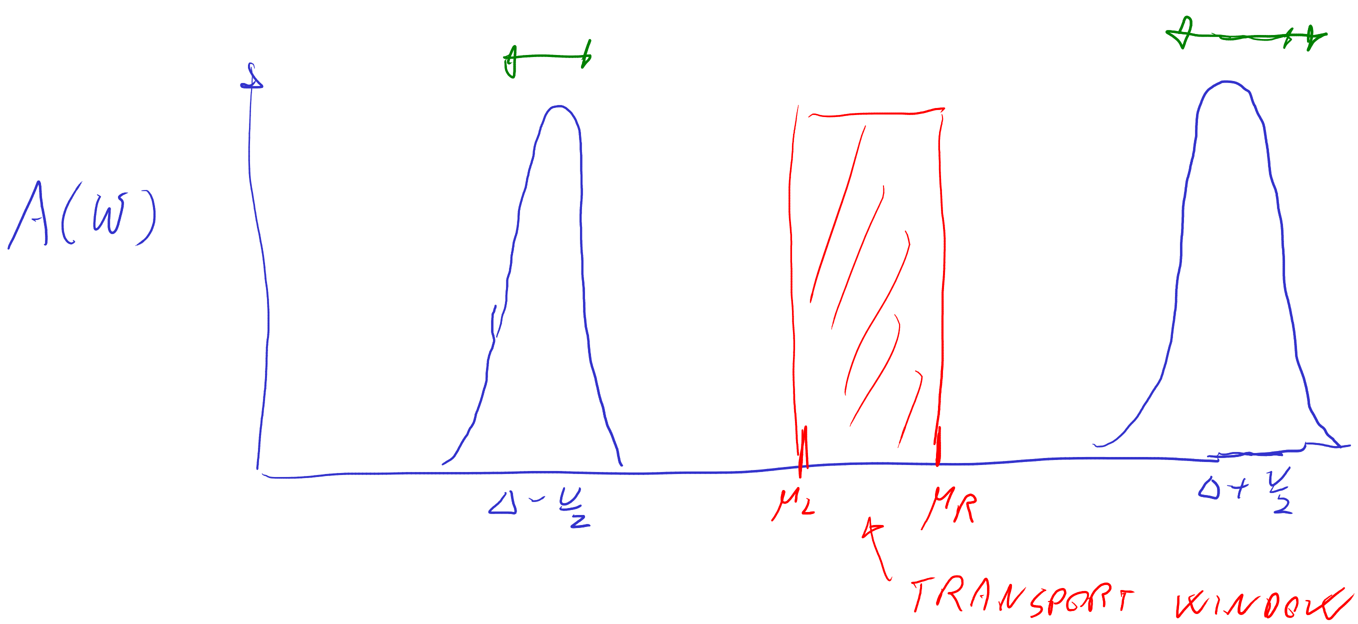
and taking the tunnel regime, for which V and thus Γ are small

we recognize that the current is strongly suppressed except when one of the resonance energies $\Delta - \frac{U}{2}$, $\Delta + \frac{U}{2}$

lies within the μ_R, μ_L

This is the Coulomb blockade effect.

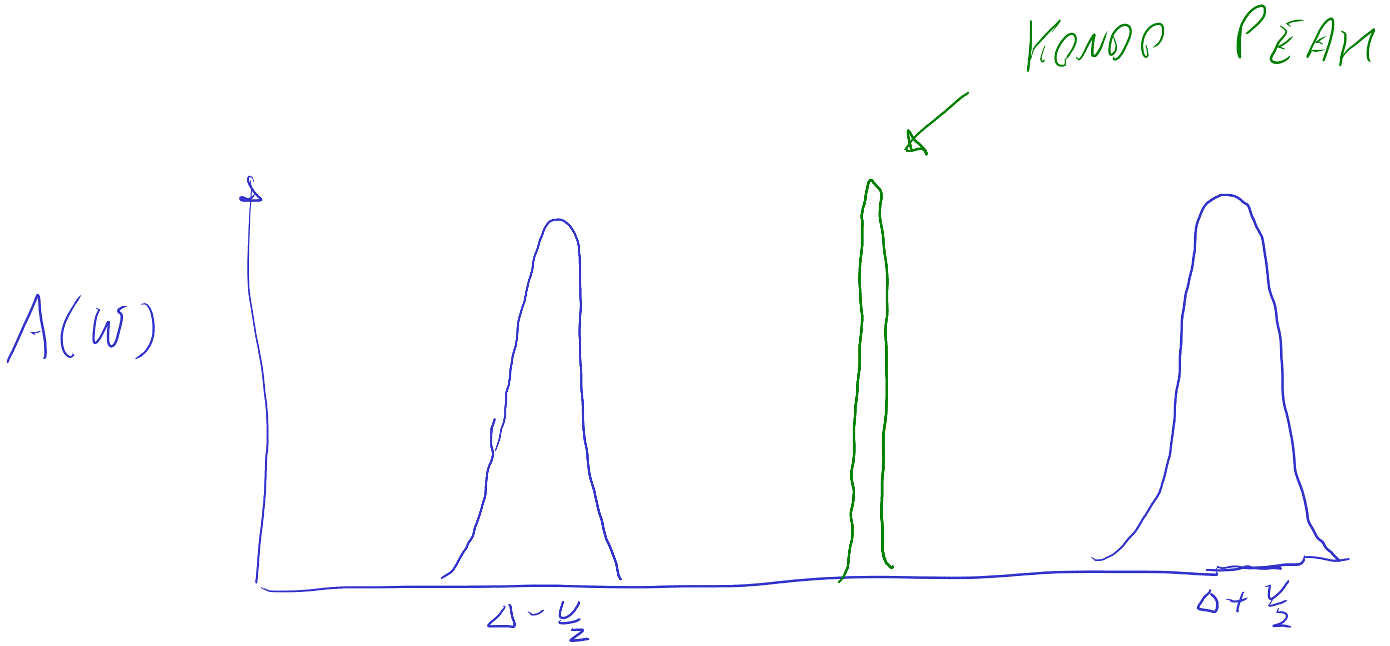
Δ = GATE VOLTAGE



This approximation is not sufficient because in the spin-degenerate case, when there is one particle, which can have spin up or down, there is resonant transmission as well.

This is due to virtual spin flip processes. Kondo effect

ONE NEEDS IMPROVED APPROXIMATIONS TO GET THIS



Time dependence for a noninteracting bath-quantum dot system

See latex file

Electron-phonon interaction

We consider a similar problem in which electrons in the central region interact with phonons only

The hamiltonian of the central region reads (we can omit spin here)

$$H_c = \Delta d^\dagger d + d^\dagger d \sum_q M_q \left(a_q^\dagger + a_q\right) + \sum_q \omega_q a_q^\dagger a_q \qquad \text{(D22)}$$

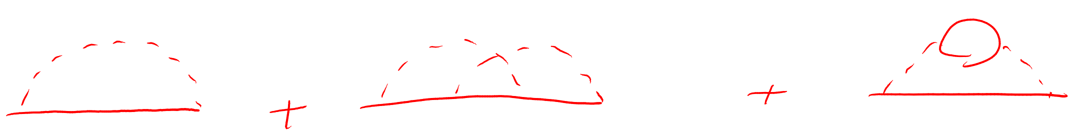
phonons

M_q, ω_q real

We consider again the approximation

$$\tilde{\Sigma} = \tilde{\Sigma}(V=0) + \times\!\sim\!\sim\!\times$$

So that $\tilde{\Sigma}(V=0)$ has an expansion



and - - - - are now phonon lines

EXACT SOLUTION OF CENTRAL REGION

THIS IS POSSIBLE BECAUSE d^+d COMMUTES WITH H_c

SO WE CAN WORK IN SEPARATE SECTORS WITH FIXED d^+d (=0,1)

IN EACH ONE, WE HAVE SIMPLE HARMONIC OSCILLATORS (shifted)

① FOR $d^+d = 0$

$$H(0) = \sum_q W_q a_q^+ a_q \qquad \text{(D23)}$$

WHOSE SOLUTION IS KNOWN

② FOR $d^+d = 1$

$$H(1) = \Delta + \sum_q M_q (a_q^+ + a_q) + \sum_q W_q a_q^+ a_q$$

DISPLACED HARMONIC OSCILLATORS

SOLVED BY $a_q = \bar{a}_q - \frac{M_q}{W_q}$

$$\Rightarrow H(1) = \Delta + \sum_q W_q \left(\bar{a}_q^+ \bar{a}_q - \cancel{(\bar{a}_q + \bar{a}_q^+)} \frac{M_q}{W_q} + \frac{M_q^2}{W_q^2} \right) + M_q \left(\cancel{\bar{a}_q + \bar{a}_q^+} - 2\frac{M_q}{W_q} \right) \Big)$$

$$= \Delta + \sum_q W_q \bar{a}_q^+ \bar{a}_q - \sum_q \frac{M_q^2}{W_q} \qquad \text{(D24)}$$

AGAIN EASY TO SOLVE

We can combine (1) and (2) by doing the transformation

$$a_q = \bar{a}_q - \frac{M_q}{W_q} d^+ d$$

and (cf. D23 D24)

$$H = \sum_q W_q \bar{a}^+_q \bar{a}_q + \left(\Delta - \sum_q \frac{M_q^2}{W_q} \right) d^+ d$$

(D25)

However, d is still not the appropriate operator, since it should not change the state of the phonons.

For example, if phonons for $d^+d = 0$ are in their ground state

$a_q|0\rangle = \bar{a}_q|0\rangle = 0$

adding an electron d^+ they are not because the harmonic oscillator is shifted

So the new d must also shift the phonons into the new ground state

Formally, this is done by a further transformation (TREATMENT: SEE MAHAN)

$$\boxed{\bar{d} = d\hat{X}}$$

$$\boxed{\hat{X} \equiv \hat{X}[\xi] = \exp\left(\sum_q \left(\xi_q a_q^\dagger - \xi_q^* a_q\right)\right) \qquad \xi_q = \frac{M_q}{\omega_q}}$$ (D26)

It has the properties (see below)

$$\boxed{\hat{X}[\xi]^\dagger a_q \hat{X}[\xi] \equiv a_q + \xi_q}$$ (D27)

* SHIFTS HARMONIC OSCILLATOR

notice that

$$\boxed{\hat{X} = \exp\left(\sum_q \left(\xi_q \bar{a}_q^\dagger - \xi_q^* \bar{a}_q\right)\right)}$$

i.e. same expression in terms of $\bar{a}_q$

Commutation rules are fullfilled

$$\{\bar{d}, \bar{d}^{+}\} = 1 \qquad [\bar{a}_q, \bar{a}_{q'}^{+}] = \delta_{qq'}$$

$$[\bar{d}, \bar{a}_q] = [d\hat{X}, a_q + \xi_q d^{+} d]$$

$$= d[\hat{X}, a_q] + \xi_q [d, d^{+} d] X$$

$$= -d\hat{X}\xi_q + \xi_q d\hat{X} = 0$$

Proof of above property

$$a_q(\xi) \equiv \hat{X}[\xi]^{+} a_q \hat{X}[\xi]$$

$$\frac{d}{d\xi_q} a_q(\xi) = \hat{X}[\xi]^{+} [a_q, a_q^{+}] \hat{X}[\xi] = 1$$

$$\Rightarrow a_q(\xi) = a_q + \xi_q \qquad \left(a_q(\xi)^{+} = a_q^{+} + \xi_q^{*}\right)$$

$$\Rightarrow a_q \hat{X}[\xi] - \hat{X}[\xi] a_q = \hat{X}[\xi] \xi_q$$

The hamiltonian becomes

$$H = \Delta \bar{d}^\dagger \bar{d} + \cancel{\bar{d}^\dagger \bar{d} \sum_q M_q (\bar{a}_q^\dagger + \bar{a}_q)}$$

$$-2 (\bar{d}^\dagger \bar{d})^2 \sum_q \frac{M_q^2}{w_q}$$

$$+ \sum_q w_q \left(\bar{a}_q^\dagger \bar{a}_q - \cancel{(\bar{a}_q + \bar{a}_q^\dagger) \frac{M_q}{w_q} \bar{d}^\dagger \bar{d}} + \frac{M_q^2}{w_q^2} (\bar{d}^\dagger \bar{d})^2 \right)$$

$$\boxed{= \bar{\Delta} \bar{d}^\dagger \bar{d} + \sum_q w_q \bar{a}_q^\dagger \bar{a}_q} \quad \boxed{\bar{\Delta} \equiv \Delta - \sum_q \frac{M_q^2}{w_q}}$$

where we have used that $(d^\dagger d)^2 = d^\dagger d$

Time dependence

$$\bar{d}(t) = \bar{d} e^{-i \bar{\Delta} t}$$

$$\bar{a}_q(t) = \bar{a}_q e^{-i w_q t}$$

$$\hat{X}(t) = \exp\left(\sum_q \left(\bar{a}_q^\dagger e^{i w_q t} \xi_q - h.c. \right) \right)$$

$$= \hat{X}[\xi_q e^{i w_q t}]$$

Use the property

$$\hat{X}[\xi]\,X[\eta] = \hat{X}[\xi+\eta]\,e^{i\,\mathrm{Im}\,\xi\eta^*}$$

$$\left(\text{use: } \quad e^A e^B = e^{A+B} e^{\frac{1}{2}[A,B]} \qquad [a^+\xi - a\xi^*, a^+\eta - a\eta^*] = \xi\eta^* - \text{c.c.} \right)$$

so that

$$d(t)\,d^+(0) = \bar{d}(t)\,\hat{X}(t)^+\,\hat{X}(0)\,\bar{d}^+(0)$$

$$\bar{d}(t)\,\bar{d}^+(0) \quad \hat{X}\left(-\xi_q e^{i\omega_q t} + \xi_q\right) e^{-i|\xi_q|^2 (\sin\omega_q t)}$$

sums over q are implicit

$$= \bar{d}(t)\,\bar{d}^+(0)\,e^{-i|\xi_q|^2 \sin\omega_q t}\,\hat{X}\left(\left(1-e^{i\omega_q t}\right)\xi_q\right)$$

$$= \underbrace{\bar{d}\,\bar{d}^{+}}_{1-\bar{d}^{+}\bar{d}}\, e^{-i(\bar{\Delta}t + \underbrace{|\xi_q|^2 \sin W_q t}_{\alpha(t)})}\, \hat{X}(\cdots)$$

$$d^{+}(0)\, d(t) = \bar{d}(0)^{+}\, \bar{d}(t)\, e^{i|\xi_q|^2 \sin W_q t}\, \hat{X}(\cdots)$$

$$= \bar{d}^{+}\bar{d}\, e^{-i(\bar{\Delta}t - i|\xi_q|^2 \sin W_q t)}\, \hat{X}(\cdots)$$

$$\{d(t), d^{+}(0)\} = \hat{X}(\cdots)\Big(e^{-i(\bar{\Delta}t+\alpha(t))} +$$

$$+ 2i\,\bar{d}\,\bar{d}^{+}\bar{d}\,\left(e^{-i\bar{\Delta}t}\sin\alpha(t)\right)\Big)$$

For definiteness we take $\bar{\Delta} > \mu$ so that the $\bar{d}$ are empty and we get

$$G^{r}_{dd}(V=0) = -i\langle\{d(t), d^{+}(0)\}\rangle\,\Theta(t)$$

$$= -i\,\Theta(t)\,\langle\hat{X}(\cdots)\rangle\, e^{-i(\bar{\Delta}t+\alpha(t))}$$

We need to evaluate

$$\langle \hat{X}(\eta) \rangle = \langle \exp(\eta \bar{a}^{+} - \eta^{*} \bar{a}) \rangle$$

for simplicity we consider a single q, since they decouple

$$= \langle \exp \eta \bar{a}^{+} \exp(-\eta^{*} \bar{a}) \exp(+\tfrac{1}{2} \eta \eta^{*} [\bar{a}^{+}, \bar{a}]) \rangle$$

For simplicity we take T=0 for which all phonons are in the ground state $\langle \bar{a}^{+} \bar{a} \rangle = 0$

$$= \exp(-\tfrac{1}{2} |\eta|^{2})$$

$$\langle \hat{X}(\underbrace{(1 - e^{-i\omega_q t}) \xi_q}_{\eta}) \rangle$$

$$= \exp\left(-\tfrac{1}{2} \sum_q |\xi_q|^2 (2 - 2\cos \omega_q t)\right)$$

$$= \exp\left(- \sum_q |\xi_q|^2 (1 - \cos \omega_q t)\right)$$

$$\langle \hat{X}(\ldots) \rangle e^{-i\alpha(t)} = \exp\left(- \sum_q |\xi_q|^2 (1 - \cos \omega_q t + i \sin \omega_q t)\right)$$

$$= \exp\left(\underbrace{- \sum_q |\xi_q|^2 (1 - e^{-i\omega_q t})}_{\Phi(t)}\right)$$

Final result:

(See also Mahan)

$$G^{r}_{dd}(V=0) = -i\,\Theta(t)\,\exp\left(-it\bar{\Delta} - \Phi(t)\right)$$

For nonzero boson occupation $N_q = f_B(\omega_q)$, one gets

$$\Phi(t) = \sum_q \frac{M_q^2}{\omega_q^2}\left(N_q\left(1-e^{i\omega_q t}\right) + \left(N_q+1\right)\left(1-e^{-i\omega_q t}\right)\right)$$

There are several interesting cases.

1) One boson

$$\Phi(t) = \frac{M_0^2}{\omega_0^2}\left(1-e^{-i\omega_0 t}\right)$$

The spectral function in ω will display peaks at the periods

i. e. a central peak at $\omega = \bar{\Delta}$ with satellite peaks at distances

of ω_0 times an integer.

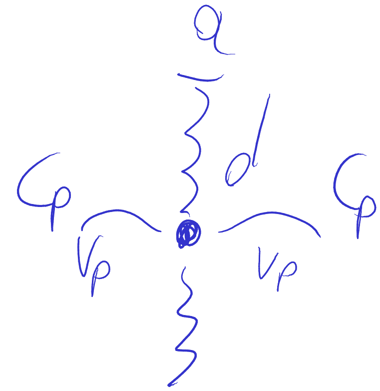
With the "Hubbard I" approximation (cf. D15A) one gets (cf. D19A)

$$\left(G(V=0)^{-1} - \sum_p V_{0p}\, g_{pp}\, V_{p0}\right)^{-1}$$

$$\tilde{\Sigma}(U=0)$$ (effect of the leads)

And, as usual the leads just broaden the peaks

Now introduce the coupling to the leads



$$\sum_p V_p c_p^\dagger d + h.c. =$$

$$= \sum_p V_p c_p^\dagger \bar{d} \hat{X}^\dagger + h.c.$$

which does no longer describe free particle due to $\hat{X}$

So this problem is not exactly solvable

In the wide-band limit, however, for which

$$\sum_p V_{0p} g^r_{pp} V_{p0} = -i\gamma$$

The C-C retarded Green's function in w independent and thus local in time

therefore when evaluating the $\bar{d}, d^\dagger$ self-energy

terms are evaluated at the same time and $\hat{X}$ cancels with $\hat{X}^\dagger$

we thus have

$$G^r_{\bar{d}\bar{d}} = \left(\left(G^r_{\bar{d}\bar{d}}(V=0)\right)^{-1} + i\gamma \right)^{-1}$$

which in real time is obtained by replacing

$$\bar{\Delta} \to \bar{\Delta} - i\gamma$$

In total, the d d retarded Green's function thus becomes

$$G^r_{dd}(V=0) = -i\,\theta(t)\,\exp\left(-it\bar{\Delta} - \Phi(t) - \gamma t\right)$$

AS USUAL, γ PRODUCES A BROADENING OF THE PHONON PEAKS

General expression for the current

$$I_\alpha = e \sum_{p \in \alpha} V_{p0} \, \mathrm{Re}\, G^K_{0p}(t=0)$$

leads

$$G_{0p} = G_{00} V_{0p} g_{pp}$$

exact

for the Keldysh component

$$G^K_{0p} = \left(G^r_{00} g^K_{pp} + G^K_{00} g^a_{pp} \right) V_{0p}$$

$$= \left(G^r_{00} \left(g^r_{pp} - g^a_{pp} \right) s_\alpha(\omega) + G^K_{00} g^a_{pp} \right) V_{0p}$$

introduce

$$-i \, \Gamma_\alpha(\omega) = \sum_{p \in \alpha} V_{0p} \underbrace{\left(g^r_{pp} - g^a_{pp} \right)}_{-2i\pi A_{pp}(\omega)} V_{p0}$$

$\propto 2\pi *$ density of states

consider two leads $\alpha = L, R$

By continuity equation $I_L = -I_R = x I_L - (1-x) I_R$

$$I_L = \int e \Big[\sum_\alpha^{L,R} \Gamma_\alpha \Delta_\alpha \eta_\alpha \, \mathrm{Im}\, G^r_{00} - \mathrm{Im}\, G^K_{00} \underbrace{\sum_p V_{0p}\, \mathrm{Im}\, g^a_{pp} V_{p0} \cdot \eta_p}_{\frac{1}{2} \sum_\alpha \eta_\alpha \Gamma_\alpha} \Big] \frac{dw}{2\pi}$$

since $\mathrm{Re}\, G^K_{00} = 0$

where
$$\eta_p = \begin{cases} x & p \in L \\ (x-1) & p \in R \end{cases}$$

$$= e \int \frac{dw}{2\pi} \Big[\mathrm{Im}\, G^r_{00} \sum_\alpha \Gamma_\alpha \Delta_\alpha \eta_\alpha - \frac{1}{2} \mathrm{Im}\, G^K_{00} \sum_\alpha \eta_\alpha \Gamma_\alpha \Big]$$

for the proportional case for which

$$\Gamma_L(\omega) = \lambda\, \Gamma_R(\omega)$$

$$I_L = e \int \frac{d\omega}{2\pi} \Big[\operatorname{Im} G_{00}^r \left(\lambda\, \gamma_L X + \gamma_R (X-1) \right) - \frac{1}{2} \operatorname{Im} G_{00}^k \big(\underbrace{\lambda X + (X-1)}_{X(1+\lambda)-1} \big) \Big] \Gamma_R$$

we can choose $$X = \frac{1}{1+\lambda}$$

so that the second term vanishes , and obtain

$$\left(\Gamma_L (1-2f_L) \frac{1}{1+\lambda} - \Gamma_R (1-2f_R) \frac{\lambda}{1+\lambda} \right)$$

$$= 2 \left(f_R - f_L \right) \Gamma_L \frac{1}{1+\Gamma_L/\Gamma_R} = 2 \left(f_R - f_L \right) \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R}$$

$$= 2e \int \frac{d\omega}{2\pi} \left(\operatorname{Im} G_{00}^r \right) \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} \left(f_R - f_L \right)$$

Fermi functions

$$= e\int \frac{d\omega}{2\pi}\, \underbrace{i\left(G^r_{00} - G^a_{00}\right)\frac{\Gamma_L\Gamma_R}{\Gamma_L+\Gamma_R}}_{\mathcal{T}(\omega)}\left(f_L - f_R\right)$$

Transmission coefficient

This expression is also valid in the presence of many orbitals in the central region. In that case one has to take the trace.

Time dependent phenomena

As an application we consider the resonant-level model

$$H_0 = \sum_p \varepsilon_p(t) c_p^\dagger c_p + \varepsilon_0(t) d^\dagger d$$

leads — central region

$$V = \sum_p V_p(t) \left(c_p^\dagger d + d^\dagger c_p \right)$$

coupling

$$c_p(t) = e^{-i\int_0^t \varepsilon_p(t')\,dt'} c_p$$

$$c_p^\dagger(t) = e^{i\int_0^t \varepsilon_p(t')\,dt'} c_p^\dagger$$

$$g_{pp}^r(t_1,t_2) \equiv -i\,\Theta(t_1-t_2) \left\langle \left\{ c_p(t_1), c_p^\dagger(t_2) \right\} \right\rangle$$

$$= -i\,\Theta(t_1-t_2)\, e^{-i\int_{t_2}^{t_1} \varepsilon_p(t')\,dt'}$$

similar for

$$g_{00}^r(t_1,t_2) = -i\,\Theta(t_1-t_2)\, e^{-i\int_{t_2}^{t_1} \varepsilon_0(t')\,dt'}$$

$$G_{00} = g_{00} + g_{00}\,\tilde{\Sigma}\,G_{00}$$

$$\tilde{\Sigma} = V_{0p}\,g_{pp}\,V_{p0}$$

Holds again provided products become time convolutions

We first evaluate

$$\tilde{\Sigma}^r(t_1,t_2) = \sum_p V_{0p}(t_1)\,g^r_{pp}(t_1-t_2)\,V_{p0}(t_2)$$

We will consider some (physically realistic) simplifications:

$$\varepsilon_p(t) = \varepsilon_p + \Delta_{\alpha_p}(t) \qquad \alpha_p = \begin{cases} L & p>0 \\ R & p<0 \end{cases}$$

$$V_{0p}(t) = V_{0p}\,u_{\alpha_p}(t)$$

consider the contributions from the two leads

$\alpha = L, R$ separately

$$\tilde{\Sigma}^r = \sum_\alpha \tilde{\Sigma}^r_\alpha$$

$$G_{00} = g_{00} + g_{00}\,\tilde{\Sigma}\,G_{00}$$

$$\tilde{\Sigma} = V_{0p}\,g_{pp}\,V_{p0}$$

Holds again provided products become time convolutions

We first evaluate

$$\tilde{\Sigma}^r(t_1,t_2) = \sum_p V_{0p}(t_1)\,g^r_{pp}(t_1,t_2)\,V_{p0}(t_2)$$

We use:

$$\varepsilon_p(t) = \varepsilon_p + \Delta_p(t)$$

$$\tilde{\Sigma}^r(t_1,t_2) = -i\sum_p V_{0p}(t_1)\;V_{p0}(t_2)\,\times$$

$$\times\; e^{-i\varepsilon_p(t_1-t_2)}\;e^{-i\int_{t_2}^{t_1}\Delta_p(t')\,dt'}\;\Theta(t_1-t_2)$$

introducing the density of states $\varrho(\varepsilon_p)$ and writing $\Delta_p(t) = \Delta(\varepsilon_p, t)$

$V_{\alpha p}(t) = V(\varepsilon_p, t)\, \mathrm{Vol}^{-\frac{1}{2}}$ as dependent of the energy

Further defining

$$2\pi\,\Gamma(\varepsilon, t_1, t_2) \equiv \varrho(\varepsilon)\, V(\varepsilon, t_1)\, V^*(\varepsilon, t_2)\, e^{-i\int_{t_2}^{t_1}\Delta(\varepsilon, t')dt'}$$

we obtain

$$\tilde{\Sigma}^r(t_1, t_2) = -i\,\Theta(t_1 - t_2)\int\frac{d\varepsilon}{2\pi}\,\Gamma(\varepsilon, t_1, t_2)\, e^{-i\varepsilon(t_1 - t_2)}$$

The last expression can be simplified in the wide-band limit.

Here we assume $\Gamma(\varepsilon, t_1, t_2)$ to be ε-independent over the range of ε relevant energies for the central region. In this limit

$$\tilde{\Sigma}^r(t_1 - t_2) = -i\,\Theta(t_1 - t_2)\,\Gamma(t_1, t_2)\,\delta(t_1 - t_2)$$

$$= -\frac{i}{2}\,\delta(t_1 - t_2)\,\Gamma(t_1)$$

$$\Gamma(t_1) \equiv \Gamma(t_1, t_1)$$

notice that there is a 1/2 factor due to the $\Theta(t_1 - t_2)\,\delta(t_1 - t_2) = \frac{1}{2}\,\delta(t_1 - t_2)$

In the wide-band limit, the self-energy becomes local in time.

$$\tilde{\Sigma}_\alpha^r(t_1,t_2) = -i\Theta(t_1-t_2)\mathcal{M}_\alpha(t_1)\mathcal{M}_\alpha^*(t_2) \times$$

$$\times\, e^{-i\int_{t_2}^{t_1}\Delta_\alpha(t')dt'} \times$$

$$\times \sum_{p\in\alpha} |V_{0p}|^2\, e^{-i\varepsilon_p(t_1-t_2)}$$

introducing the density of states $\varrho(\varepsilon_p)$ and writing $V_{0p} = V(\varepsilon_p)\,\mathrm{vol}^{-\frac{1}{2}}$ as dependent of the energy

Further defining

$$\boxed{2\pi\,\Gamma_\alpha(\varepsilon,t_1,t_2) \equiv \mathcal{M}_\alpha(t_1)\mathcal{M}_\alpha^*(t_2)\, e^{-i\int_{t_2}^{t_1}\Delta_\alpha(t')dt'} \times |V(\varepsilon)|^2\varrho(\varepsilon)}$$

$$\boxed{\tilde{\Sigma}_\alpha^r(t_1,t_2) = -i\,\Theta(t_1-t_2)\int\frac{d\varepsilon}{2\pi}\,\Gamma_\alpha(\varepsilon,t_1,t_2)\,e^{-i\varepsilon(t_1-t_2)}}$$

The last expression can be simplified in the wide-band limit. Here we assume $\Gamma_\alpha(\varepsilon,t_1,t_2)$ to be ε independent over the range of ε relevant energies for the central region. In this limit

$$\tilde{\Sigma}_\alpha^r(t_1-t_2) = -i\,\Theta(t_1-t_2)\,\Gamma_\alpha(t_1,t_2)\,\delta(t_1-t_2)$$

$$= -\frac{i}{2}\,\delta(t_1-t_2)\,\Gamma_\alpha(t_1)$$

The Dyson equation now becomes

$$\propto \delta(t_3 - t_4)$$

$$G^r_{00}(t_1,t_2) = g^r_{00}(t_1,t_2) + \int g^r_{00}(t_1,t_3)\tilde{\Sigma}^r(t_3,t_4)\, G^r_{00}(t_4,t_2)\, dt_3 dt_4$$

$$= g^r_{00}(t_1,t_2) - \frac{i}{2}\int dt_3\, g^r_{00}(t_1,t_3)\,\Gamma(t_3)\, G^r_{00}(t_3,t_2)$$

This is best transformed into a differential equation by multiplying by $\left(g^r_{00}\right)^{-1}$ from the left

$$\left(g^r_{00}\right)^{-1}(w) = w - \varepsilon_0 \Rightarrow$$

$$\left(g^r_{00}\right)^{-1}(t_1,t_2) = \delta(t_1 - t_2)\left(i\frac{\partial}{\partial t_2} - \varepsilon_0(t_2)\right)$$

It is instructive to check that

$$\left(g^r_{00}\right)^{-1} \circledast g^r_{00} = I$$

$$\int dt_2 \left(g^r_{00}\right)^{-1}(t_1,t_2)\, g^r_{00}(t_2,t_3) = \delta(t_1 - t_3)$$

we now leave this implicit (Einstein summation convention)

$$\delta(t_1-t_2)\left(i\frac{\partial}{\partial t_2}-\varepsilon_0(t_2)\right)g_{00}^r(t_2,t_3)\overset{?}{=}I=\delta(t_1-t_3)$$

apply to

$$g_{00}^r(t_2,t_3)=-i\Theta(t_2-t_3)\,e^{-i\int_{t_3}^{t_2}\varepsilon_0(t')dt}$$

$$\delta(t_1-t_2)\Big(\delta(t_2-t_3)-i\Theta(t_2-t_3)\times$$

$$\big(\varepsilon_0(t_2)-\varepsilon_0(t_2)\big)\Big)e^{-i\int_{t_3}^{t_2}\varepsilon_0(t')dt'}$$

$$=\delta(t_1-t_3)$$

Now let us apply it to the Dyson equation

first formally

$$g_{00}^{r\,-1}G_{00}^r=I-\frac{i}{2}\Gamma G_{00}^r$$

$$\left(g_{00}^{r\,-1}+\frac{i}{2}\Gamma\right)G_{00}^r=I$$

$$\delta(t_1-t_2)\left(i\frac{\partial}{\partial t_2}-\varepsilon_0(t_2)+\frac{i}{2}\Gamma(t_2)\right)G^r_{00}(t_2,t_3)$$

$$=\delta(t_1-t_3)$$

so it's now easy to guess the solution: it has the same shape as g^r_{00} with the replacement $\varepsilon_0 \to \varepsilon_0 - \frac{i}{2}\Gamma$

$$\boxed{G^r_{00}(t_1,t_2) = -i\,\Theta(t_1-t_2)\,e^{-i\int_{t_2}^{t_1}\left(\varepsilon_0(t')-\frac{i}{2}\Gamma(t')\right)dt'}}$$

The advanced Green's function is quite generally given by

$$G^a_{00}(t_1,t_2) = G^r_{00}(t_2,t_1)^* =$$

$$= i\,\Theta(t_2-t_1)\,e^{-i\int_{t_2}^{t_1}\left(\varepsilon_0(t')+\frac{i}{2}\Gamma(t')\right)dt'}$$

we now need the Keldysh Green's function

warning, if initial condition have to be taken into account the g_k term has to be considered

$$G^K = G^r \tilde{\Sigma}^K G^a$$

$$G^K(t_1,t_2) = \int dt_3 dt_4\, G^r(t_1,t_3)\tilde{\Sigma}^K(t_3,t_4)G^a(t_4,t_2)$$

$$\tilde{\Sigma}^K(t_1,t_2) = \sum_p V_{0p}(t_1)\left(g^r_{pp}(t_1,t_2) - g^a_{pp}(t_1,t_2)\right) h_{\alpha_p}(\varepsilon_p)\, V_{p0}(t_2)$$

here we have taken into account the fact that the distribution

functions $h_{\alpha_p}(\varepsilon_p)$ are fixed at some constant energies

in the past

$$\left(g^r_{pp}(t_1,t_2) - g^a_{pp}(t_1,t_2)\right) = -i\, e^{-i\int_{t_2}^{t_1}\varepsilon_p(t')\,dt'}$$

$$\tilde{\Sigma}^K(t_1,t_2) = \sum_{\alpha=L,R} \tilde{\Sigma}^K_\alpha(t_1,t_2)$$

$$\tilde{\Sigma}^K_\alpha(t_1,t_2) = \sum_{p\in\alpha} V_{0p}(t_1)\, V_{p0}(t_2)\, e^{-i\int_{t_2}^{t_1}\Delta_p(t')\,dt'}$$

$$\times\, e^{-i\varepsilon_p(t_1-t_2)}\, h_\alpha(\varepsilon_p) \quad (-i)$$

$$= -i \int \frac{d\varepsilon}{2\pi}\, \Gamma_\alpha(\cancel{\varepsilon}, t_1, t_2)\, e^{-i\varepsilon(t_1-t_2)}\, \Lambda_\alpha(\varepsilon)$$

where we have introduced the same definition for Γ as above, just separated for the two leads

due to the $\Lambda_\alpha(\varepsilon)$ this does not simplify into a $\delta(t_1-t_2)$ in the wide-band limit (WBL)

$$G^n_{00}(t_1,t_2) = -i \int_{-\infty}^{t_1} dt_3\, e^{-i\int_{t_3}^{t_1}\left(\varepsilon_0(t') - \frac{i}{2}\Gamma(t')\right)dt'} \int_{-\infty}^{t_2} dt_4\, e^{-i\int_{t_2}^{t_4}\left(\varepsilon_0(t') + \frac{i}{2}\Gamma(t')\right)dt'}$$

$$\sum_\alpha \int \frac{d\varepsilon}{2\pi}\, \Gamma_\alpha(t_3, t_4)\, e^{-i\varepsilon(t_3-t_4)}\, \Lambda_\alpha(\varepsilon)$$

There is no further simplification at this point in the WBL due to the energy dependence of Λ_α

$(-i \;\; ?)$

The current

$$I_\alpha = e \sum_{p\in\alpha} V_{p0} \, \mathrm{Re}\, G^K_{0p}(t=0)$$

leads

$$\sum_{p\in\alpha} V_{p0} G^K_{0p}(t,t) =$$

$$\sum_{p\in\alpha}\int dt' \, V_{p0}\left(G^r_{00}(t,t')\, g^K_{pp}(t',t) + G^K_{00}(t,t')\, g^a_{pp}(t',t)\right) V_{0p}$$

$$= \int dt' \left(G^r_{00}(t,t')\, \tilde{\Sigma}^K_\alpha(t',t) + G^K_{00}(t,t')\, \tilde{\Sigma}^a_\alpha(t',t)\right)$$

At this point there is only a little reshuffling and tedious transformations

The result is given in Jauho's book as

$$I_\alpha = -e\left[\Gamma_\alpha(t)\, N(t) + \int \frac{d\varepsilon}{\pi} f_\alpha(\varepsilon) \times \int_{-\infty}^{t} dt_1\, \Gamma_\alpha(t_1,t)\, \mathrm{Im}\left(e^{-i\varepsilon(t_1-t)}\, G^r(t,t_1)\right)\right]$$

$$I_\alpha = -e\,\Gamma_\alpha |u_\alpha(t)|^2 N(t)$$

$$-e\,\Gamma_\alpha\, u_\alpha(t) \int \frac{d\varepsilon}{\pi} f_\alpha(\varepsilon)\, \mathrm{Im}\, A_\alpha(\varepsilon,t)$$

where a homogeneous time dependent is assumed

$$V_{\alpha p}(t) = u_{\alpha_p}(t)\, V_{\alpha p} \Rightarrow \Gamma_\alpha(t) = \Gamma_\alpha |u_\alpha(t)|^2$$

where the particle number in the central region:

$$N(t) = \mathrm{Im}\, G^<(t,t) =$$

$$= \sum_\alpha \Gamma_\alpha \int \frac{d\varepsilon}{2\pi} f_\alpha(\varepsilon) |A_\alpha(\varepsilon,t)|^2$$

we have introduced

$$A_\alpha(\varepsilon,t) = \int dt_1\, u_\alpha(t_1)\, G^r(t,t_1)$$

$$\exp\left(i\varepsilon(t-t_1) - i\int_t^{t_1} dt_2\, \Delta_\alpha(t_2)\right)$$

THE END

we evaluate the last integral at zero temperature for which

$$S_\alpha(\varepsilon) = 1 - 2 f_F(\varepsilon - \mu_\alpha) = \mathrm{sign}(\varepsilon - \mu_\alpha)$$

$$\int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \, e^{-i\varepsilon\tau} \, \mathrm{sign}(\varepsilon - \mu) =$$

$$= e^{-i\mu\tau} \left(\int_0^\infty e^{-i\varepsilon(\tau - i\delta)} \frac{d\varepsilon}{2\pi} - \int_0^\infty e^{i\varepsilon(\tau + i\delta)} \frac{d\varepsilon}{2\pi} \right)$$

$$= e^{-i\mu\tau} \frac{1}{2\pi} \left(\frac{1}{i(\tau - i\delta)} - \frac{1}{-i(\tau + i\delta)} \right)$$

$$-i \, e^{-i\mu\tau} \frac{1}{2\pi} \left(\frac{1}{\tau - i\delta} + \frac{1}{\tau + i\delta} \right)$$

$$= -\frac{i}{\pi} e^{-i\mu\tau} \, P \frac{1}{\tau}$$

$$\tilde{\Sigma}_\alpha^{r}(t_1, t_2) =$$

$$-i \frac{\gamma}{\pi} M_\alpha(t_1) M_\alpha(t_2)^* \, e^{-i \int_{t_2}^{t_1} \Delta_\alpha(t') dt'} \, e^{-i\mu(t_1 - t_2)} \, P \frac{1}{t_1 - t_2}$$

However, we will see
that the problem remains exactly solvable in the
"wide-band" limit, which corresponds to the
Markovian limit

This occurs when the energy scale of the leads is
much larger than the energy scales of the central region.

This is equivalent to say that the time scales of the leads
are much faster than the ones of the central region

In that case the response is istantaneous, so that
only equal-time (t=0) Green's functions are affected.
These are the same for d, $\bar{d}$

DEF $\quad \bar{G}(t) = G^R_{\bar{d}\bar{d}}(t) = -i\,\Theta(t)\langle\{\bar{d}(t), \bar{d}(0)^\dagger\}\rangle$

$$i\frac{\partial}{\partial t}\bar{G}(t) = \frac{\partial}{\partial t}\Theta(t)\langle\{\bar{d}(t), \bar{d}(0)^\dagger\}\rangle$$

$$= \delta(t)\,\bar{G}(t) + i\,\Theta(t)\langle\{[H, \bar{d}(t)], \bar{d}(0)^\dagger\}\rangle$$

$$[H, \bar{d}(t)] = -\bar{\Delta}\,\bar{d}(t) - \sum_p X(t)\,c_p(t)$$
$$\bar{d}^\dagger(t)\,c_p(t)\,X(t)$$

$$= \delta(t)\,\bar{G}(t) - i\,\bar{\Delta}\,\bar{G}(t)$$
$$-i\,\Theta(t)\langle X(t)\{c_p(t), \bar{d}(0)\}\rangle$$

$$H_p = \varepsilon_p c_p^\dagger c_p + V_p \left(c_p^\dagger d + h.c. \right)$$

$$i G_{pd} \equiv \theta(t) \left\langle \left\{ c_p(t), d^\dagger(0) \right\} \right\rangle$$

$$i \dot{G}_{pd} = \delta(t) G_{pd} + i\theta(t) \left\langle \left\{ \underbrace{[H, c_p(t)]}_{-\varepsilon_p c_p - V_p d}, d^\dagger \right\} \right\rangle$$

$$= \underbrace{\delta(t)}_{=0} G_{pd} \underbrace{- i\theta(t) \left\langle \left\{ d(t), d^\dagger \right\} \right\rangle}_{G_{dd}(t)} V_p$$

$$\underbrace{- i\theta(t) \left\langle \left\{ c_p(t), d^\dagger \right\} \right\rangle}_{G_{pd}} \varepsilon_p$$

$$(i\partial_t - \varepsilon_p) G_{pd} = V_p G_{dd}$$

$$G_{pd}(t=0) = 0$$

$$G_{pd} = e^{-i\varepsilon_p t} \bar{G}_{pd}$$

$$e^{-i\varepsilon_p t} (\cancel{\varepsilon_p} + i\partial_t - \cancel{\varepsilon_p}) \bar{G}_{pd} = V_p G_{dd}$$

$$i\bar{G}_{pd}(t) = \int_0^t e^{i\varepsilon_p t'} V_p G_{dd}(t') dt'$$

$$i G_{pd}(t) = \int_0^t e^{i\varepsilon_p (t'-t)} V_p G_{dd}(t') dt'$$

$$(\varepsilon_p \to \varepsilon_p - i0^+)\,?$$

$$i\,\partial_t G_{dd}(t)\Big|_{\text{FROM } p} = i\,\Theta(t)\left\langle \left\{ \underbrace{\left[H_p, d\right]_t}_{-V_p c_p}, d^\dagger(0) \right\} \right\rangle$$

$$= V_p\, G_{pd}(t)$$

$$\sum_p V_p G_{pd}(t) = -i \sum_p V_p^2 \int_0^t e^{i\varepsilon_p (t'-t)} G_{dd}(t')\, dt'$$

$$\sum_p = \mathrm{vol} \int g(\varepsilon_p)\, d\varepsilon_p$$

wide-band limit: $V_p^2\, g(\varepsilon_p) = \dfrac{\gamma}{\pi\,\mathrm{vol}}$ is approximately constant in a large energy range. Specifically, it changes only over energies much larger than the typical energies of the central region.

$$-2i\gamma \int_0^{t'} \delta(t-t')\, G_{dd}(t')\, dt'$$

The integration over $\delta(t-t')dt'$ gives just $\frac{1}{2}$, because it's at the border

$$\frac{\partial}{\partial t} G_{dd}(t)\Big|_{\text{FROM ALL } p} = -\gamma\, G_{dd}(t)$$

It is instructive to see everything in frequency space:

$$i\frac{\partial}{\partial t} \to \omega$$

$$(\omega - \varepsilon_p)\, G_{pd} = V_p\, G_{dd}$$

$$\omega\, G_{dd} = \sum_p V_p\, G_{pd} \quad + \text{ d-d contribution}$$

$$= \sum_p V_p^2 \frac{1}{\omega - \varepsilon_p + i0^+} G_{dd} + \text{ d-d contribution}$$

the $+i0^+$ is due to the fact that we have retarded Green's functions

In the wide-band limit

$$\sum_p V_p^2 \frac{1}{\omega - \varepsilon_p + i0^+} \approx \text{vol} \int V_p^2\, g(\varepsilon_p)\, d\varepsilon_p \frac{1}{\omega - \varepsilon_p + i0^+}$$

$$\approx \frac{\gamma}{\pi} \int d\varepsilon \frac{1}{\omega - \varepsilon + i0^+} = \frac{\gamma}{\pi} \int d\varepsilon \left(P\frac{1}{\omega - \varepsilon} - i\pi\delta(\omega - \varepsilon) \right)$$

$$= -i\gamma$$ independent of ω i.e. $\propto \delta(t-t')$ in real time

$$i\partial_t \langle T\, d(t) X(t) \quad X^\dagger(0)\, d^\dagger(0) \rangle$$

$$d \qquad \bar{d}$$

$$G = g + g\Sigma G$$

$$\Sigma = G^{-1} - g^{-1}$$

Functional integral

$$\bar{d}^+ X^+ \frac{\partial}{\partial t} \bar{d} X = d^+ \frac{\partial}{\partial t} d + \bar{d}^+ X^+ \bar{d} \frac{\partial}{\partial t} X$$

$$\bar{d}^+ \bar{d} \frac{\partial}{\partial t} \log X \to \bar{d}' \bar{d} \frac{\partial}{\partial t} (\xi a^+ - \xi^* a)$$

$$\bar{a}^+ \frac{\partial}{\partial t} \bar{a} = X^+ a^+ X \frac{\partial}{\partial t} X^{-1} a X$$

$$(\bar{a}^+ - \xi d^+ d) \frac{\partial}{\partial t} (\bar{a} - \xi^* d^+ d)$$

$$\bar{a}^+ \frac{\partial}{\partial t} a - \xi d^+ d \frac{\partial}{\partial t} a + \xi^* d^+ d \frac{\partial}{\partial t} a^+$$

Todo

3) relation to master equation
4) Time dependence