UNTIL HERE 6.APR.2011

We will now treat some simple examples in steady state

1) Switching on a diagonal potential at $t = t_0$

$$H_0 = \sum_p \varepsilon_p c_p^\dagger c_p$$

we take fermions

$$\hat{V} = \theta(t - t_0) \sum_p V_p c_p^\dagger c_p$$

the steady state of course occurs at a time far away from t_0

$$\Sigma(p, w) = V_p \cdot I_{2x2}$$

Dyson's equation

$$G = G_0 + G_0 * \Sigma * G$$

$$G^{-1} = G_0^{-1} - \Sigma$$

This equation is valid in general as solution of the integral equation, provided one carries out the inversions in the appropriate space, which could be the space of quantum numbers or possible time, as well as of course Keldysh space

Since there is time translation invariance, we can transform into frequency space, in which G are diagonal. In addition, in this problem they are also diagonal in quantum number space , so we need just to invert in 2x2 Keldysh space

In order to limit indices, we will denote by small g the unperturbed Green's functions

$$G_0 \equiv g = \left(\begin{array}{c|c} g_r & g_k \\ \hline & g_a \end{array} \right)$$

We don't specify the index p, since expressions are the same for all p

$$g^{-1} = \left(\begin{array}{c|c} g_r^{-1} & -g_r^{-1} g_a^{-1} g_k \\ \hline & g_a^{-1} \end{array} \right)$$

Let us inspect the Keldysh part of the inverse Green's function

$$-g_r^{-1} g_a^{-1} g_K = 2\pi i \left(W - \varepsilon_p + i\delta\right)\left(W - \varepsilon_p - i\delta\right)\delta(W-\varepsilon_p)\, n(W)$$

This object is in principle zero since

$$(W - \varepsilon_p) \cdot \delta(W - \varepsilon_p) = 0$$

and $\delta \to 0^+$

The point is that the problem is ill defined since time dependence is periodic, so the steady state can never be reached unless one introduces some dissipation mechanism.
This can be formally provided by taking δ to be a small but finite quantity and taking $\delta \to 0^+$ only at the end

Of course we should not forget that also $\delta(w-\varepsilon_p)$ becomes a lorentian curve for nonzero δ

At best we work with the general expression

$$g_k = (g_r - g_a)\, 2(w)$$

so that $$(g^{-1})_k = -(g_a^{-1} - g_r^{-1})\, 2(w)$$

$$G = (g^{-1} - \Sigma)^{-1} \equiv \left(\begin{array}{c|c} G_r & G_k \\ \hline & G_a \end{array}\right)$$

$$= \left(\begin{array}{c|c} g_r^{-1} - V_p & (g^{-1})_k \\ \hline & g_a^{-1} - V_p \end{array}\right)^{-1}$$

$$G_r = (g_r^{-1} - V_p)^{-1} = (w - \varepsilon_p - V_p + i\delta)^{-1}$$

As expected, this is the retarded Green's function of the total Hamiltonian $H_0 + V(\infty)$

$$G_a = G_r^*$$

$$G_K = - G_R G_A \left(\mathcal{J}^{-1}\right)_K$$

$$= G_R G_A \left(\mathcal{J}_A^{-1} - \mathcal{J}_R^{-1}\right) \lambda(W)$$

Since $\mathcal{J}_A^{-1} - \mathcal{J}_R^{-1} = G_A^{-1} - G_R^{-1}$

$$= \left(G_R - G_A\right) \lambda(W)$$

Now, this result is NOT what we would have expected!
It tells us, that the chemical potential contained in

$$\lambda(W) = \operatorname{sign}(W - \mu)$$

has not changed. This means that, for example, if

$V > 0$ the number of particles has decreased!

Where have the particles gone?
The point is that by taking a nonzero δ

we assumed a small interaction with some environment.
This is necessary, otherwise the system cannot reach the steady state.
The particles have thus leaked into the environment!

We will see this issue more in detail later
The point is that we take two limits

$t \to \infty$ and $\delta \to 0$

and these have to be carried out in this order.

But let us now evaluate the particle number
(we can evaluate the particle number for each p)

For this we have to use a relation valid in general
(not only for equilibrium Green's functions)

$$G_H(t) = G^{>}(t) + G^{<}(t)$$

for t=0

$$G_H(p,p',t=0) = -i \langle c_p c_{p'}^{+} - c_{p'}^{+} c_p \rangle$$

$$= 2i \langle c_{p'}^{+} c_p \rangle - i\delta_{pp'}$$

$$\langle c_{p'}^{+} c_p \rangle = -\frac{i}{2} G_H(p,p',t=0) + \frac{1}{2}\delta_{pp'}$$

$$= -\frac{i}{2} \int \frac{dw}{2\pi} G_H(p,p',w) + \frac{1}{2}\delta_{pp'}$$

Which is an expression we will use often (B-1)

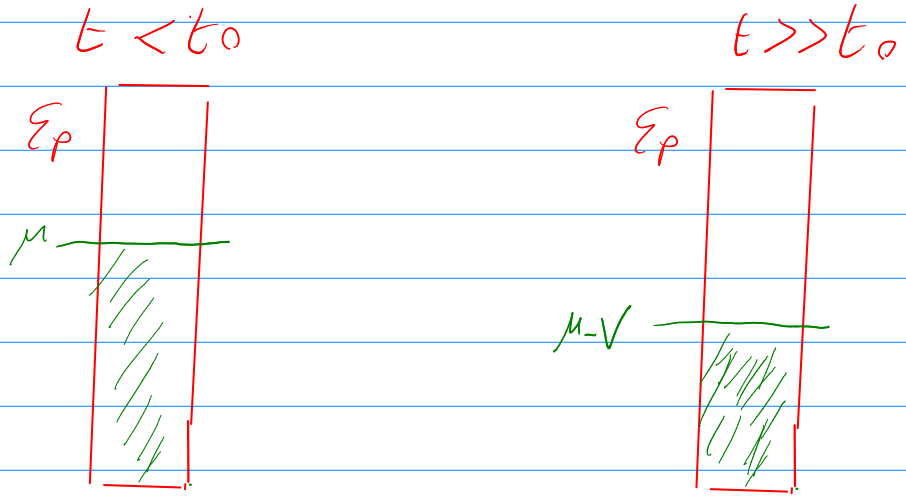
For our problem

$$\langle c_p^\dagger c_p \rangle = -\frac{i}{2} \int \frac{dw}{2\pi} \left(G_R - G_A \right) \Delta(w) + \frac{1}{2}$$

$$G_R - G_A = -2\pi i \, \delta(w - \varepsilon_p - V)$$

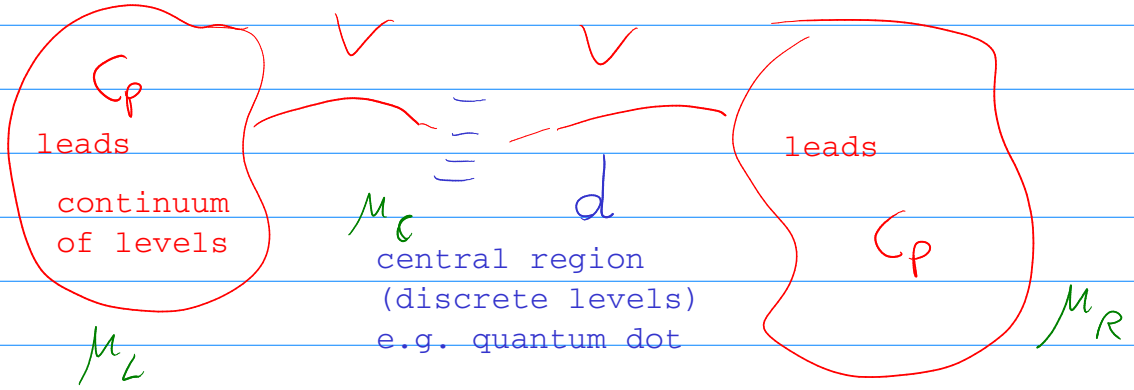
$$\frac{1}{2}\left(-\Delta(\varepsilon_p + V) + 1 \right) = \Theta\left(\mu - (\varepsilon_p + V) \right)$$

Histogram of occupied states



Noninteracting resonant level model

Description of mesoscopic tunneling structures



At t< t0 V=0, each region is in equilibrium
generally with different chemical potentials μ_L, μ_R, μ_C

Of course if the chemical potentials
of the two leads are different, we espect a current to
flow. We also espect that the chemical potential of the central
region (initial state), being a system with few degrees of freedom
does not play a role in the steady state.

We start with a problem with a single lead. In that case we
espect the central region to end up to equilibrate with the
contact with, say, $\mu = \mu_L$

For simplicity, we consider here the case in which the central region has only one level. The extension to many levels is straightforward

$$H_0 = \sum_p \epsilon_p c_p^+ c_p + \Delta\, d^+ d$$

leads — central region

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

coupling

In this case , the different p level mix up, so that one must in principle invert a "big" matrix

Time translation invariance is still valid, so we can work in frequency space.

Dyson's equation can be written for each w

$$G = \mathcal{G} + \mathcal{G} V G$$

where this has to be seen as a matrix equation

In index notation we can write it as

$$G_{qq_1} = \mathcal{G}_{qq_1} + \mathcal{G}_{qq_2} V_{q_2 q_3} G_{q_3 q_1}$$

where the index q can refer to a p or to 0 (associated with the d-level).
Double (i.e. internal) indices are summed over.

For each couple of indices each term is a 2x2 matrix in Keldysh space, for example

$$G_{qq_1} = \left(\begin{array}{c|c} G^r_{qq_1} & G^k_{qq_1} \\ \hline & G^a_{qq_1} \end{array} \right)$$

We can now exploit the fact that the $\mathcal{G}$ are diagonal, and that $V_{q_2 q_3}$ is nonzero only when one of the two q is 0:

We write two equations for the central region and for the connections

$$G_{00} = g_{00} + g_{00} V_{0p} G_{p0}$$

$$G_{p0} = \cancel{g_{p0}} + g_{pp} V_{p0} G_{00}$$

where $p \neq 0 \Rightarrow$

$$G_{00} = g_{00} + g_{00} V_{0p} g_{pp} V_{p0} G_{00} \qquad \text{(B2)}$$

This has the same form as a (closed) Dyson equation for the environment, whit an "effective" self-energy

$$\tilde{\Sigma} = V_{0p} g_{pp} V_{p0} \qquad \text{(B3)}$$

The solution is again

$$G_{00} = \left(g_{00}^{-1} - \tilde{\Sigma} \right)^{-1}$$

Remember, each one is a 2x2 matrix in Keldysh space.
In fact this matrix form can be straightfowardly applied to the case in which the central regions are many levels.
In that case the various matrices with index 0 refer to many levels as well

With the help of the "useful relations" we recognize that the retarded and advanced Green's function do not mix.
Therefore we have

$$G_{00}^{r} = \left((g_{00}^{r})^{-1} - \tilde{\Sigma}^{r} \right)^{-1}$$

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

And the same for the advanced part

Where we have used the fact that V is diagonal in Keldysh space

The Keldysh GF is somewhat different

Using the expression for the inversion, we obtain

$$G_{00}^{K} = - G_{00}^{r} \left(g_{00}^{-1} - \tilde{\Sigma} \right)^{K} G_{00}^{a}$$

with

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

$$\left(g_{00}^{-1} \right)^{K} = - g_{00}^{r\,-1}\, g_{00}^{K}\, g_{00}^{a\,-1}$$

$$= - g_{00}^{r\,-1} \left(g_{00}^{r} - g_{00}^{a} \right) g_{00}^{a\,-1}\, \lambda(w)$$

$$= \left(g_{00}^{r\,-1} - g_{00}^{a\,-1} \right) \lambda_c(w)$$

where $\lambda_c(w) = \mathrm{sign}(w - \mu_c)$

Again this term is in principle zero for a system with a finite number of degrees of freesom. Formally

$$\left(g_{00}^{r-1} - g_{00}^{a-1}\right) = 2i\delta \qquad (\delta \to 0^+)$$

However, in this case, we can see that this term can be often set to zero.

In particular it can be safely set to zero
1) When G^a, G^r are nonsingular for frequencies on the real axis

as we shall see, this is often the case here

OR
2) When $\tilde{\Sigma}$ is nonzero, in that case it "shadows" the small imaginary part

As one can see, the "initial conditions" for the central region expressed by its chemical potential μ_C do not affect its Green's function in the steady state. This makes physically sense, since the steady state takes place after a long time and the central region is finite.

We thus have

$$G_{00}^{K} = G_{00}^{r} V_{0p} g_{pp}^{K} V_{p0} G_{00}^{a} \qquad \text{(B4)}$$

To make some progress we take $V_{0p} = V$ independent of p

$$\sum_p \left(g_{pp}^{r} - g_{pp}^{a}\right) = -2i\pi \sum_p \delta(w - \varepsilon_p) = -2i\pi \rho_L^0(w)$$

where $\rho_L^0(w)$ is the density of states of the uncoupled lead, which is a continuous function of w provided the environment is infinite.

$$\sum_p g_{pp}^{K} = -2i\pi \rho_L^0(w) f_L(w) \qquad \text{(B5)}$$

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$$G_{00}^{K} = -2i\pi V^2 \left| G_{00}^{r}(w) \right|^2 \varrho_L^0(w)\, n_L(w) \qquad \text{(B6)}$$

where we have used the fact that

$$G_{00}^{r} = G_{00}^{a\,*}$$

The retarded GF is obtained as

$$G_{00}^{r} = \left(g_{00}^{r\,-1} - V_{0\rho}\, g_{\rho\rho}^{r}\, V_{\rho 0} \right)^{-1}$$

$$= \left(w - \Delta + i\delta - V^2 \sum_{\rho} g_{\rho\rho}^{r} \right)^{-1}$$

$$\sum_{\rho} g_{\rho\rho}^{r} = \underbrace{\mathrm{Re} \sum_{\rho} g_{\rho\rho}^{r}}_{\equiv R(w)} + i\, \underbrace{\mathrm{Im} \sum_{\rho} g_{\rho\rho}^{r}}_{\frac{1}{2}\sum_{\rho}\left(g_{\rho\rho}^{r} - g_{\rho\rho}^{a}\right) = -i\pi\, \varrho_L^0(w)} \qquad \text{(B6A)}$$

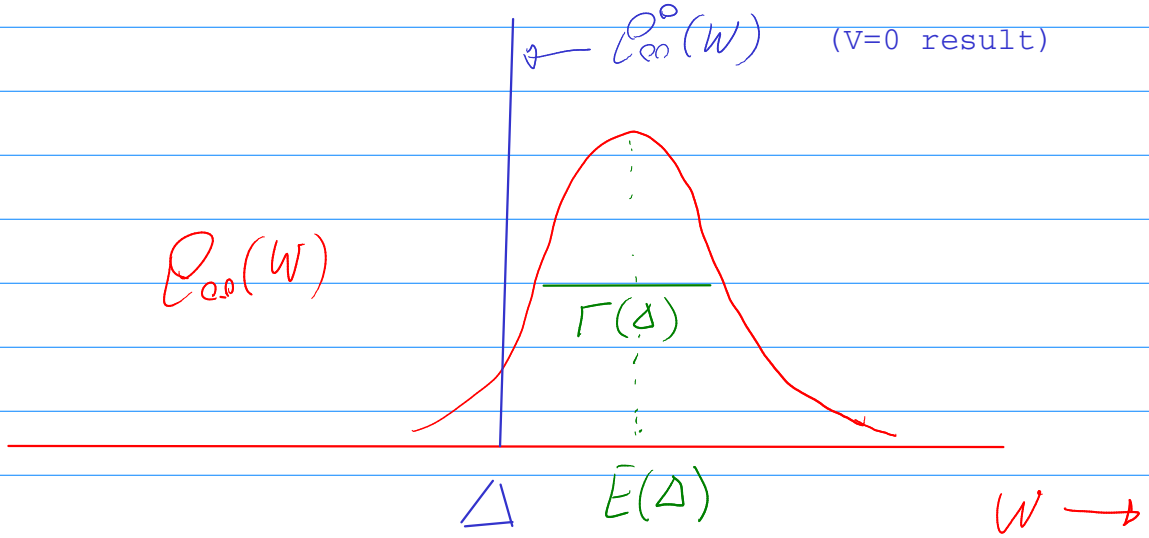
$$= \Big(w - \overbrace{\left(\Delta + V^2 R(w)\right)}^{E(w)} + i\, \overbrace{\pi V^2 \varrho_L^0(w)}^{\Gamma(w)} \Big)^{-1} \qquad \text{(B6B)}$$

where δ can be neglected, since the coupling to the environment provides a finite imaginary part

The imaginary part provides a broadening of the spectral function (local density of states) $\sim \Gamma(\Delta)$

and R gives a shift of the level $\simeq V^2 R(\Delta)$

$$\rho_{00}(w) = -\frac{1}{\pi} \operatorname{Im} G^r_{00}(w)$$



With the expression $$G^r_{00} = \frac{1}{w - E(w) + i\Gamma(w)}$$

we can write

$$G^r_{00} - G^a_{00} = \frac{-2i\Gamma(w)}{(w-E(w))^2 + \Gamma(w)^2} = -2i\Gamma(w)\left|G^r_{00}(w)\right|^2$$

$$= -2i\pi V^2 \rho_L(w)\left|G^r_{00}(w)\right|^2 \qquad \text{(B6C)}$$

so that the Keldysh Green's function assumes a form similar to the uncoupled case

$$G^K_{00} = \left(G^r_{00} - G^a_{00}\right) \mathcal{F}_L(w) \qquad \text{(B7)}$$

This is of course expected, since for the case of a single lead the steady state is an equilibrium state.

The above equation tells us that the central region equilibrates and its distribution is controlled by the initial distribution function $\mathcal{D}_L(W)$ of the lead. In other words the central region acquires

the same chemical potential and temperature (both are included in $\mathcal{D}_L$ only) of the lead.

$$\mathcal{D}_L(W) = 1 - 2n(W) = 1 - 2f_F(W - \mu_L)$$

for fermions, where f_F is the Fermi function

The more interesting case of two leads can be easily obtained by formally extending the above results.

We can, for example, associate the states of the Left lead with p<0 and the ones of the right one to p>0

Everything is identical, except that the leads now have

two different distribution functions ϱ_L, ϱ_R, therefore (cf B5)

$$\sum_p \gamma_{pp}^{K} = -2i\pi\left(\varrho_L^0(W)\,\mathcal{D}_L(W) + \varrho_R^0(W)\,\mathcal{D}_R(W)\right)$$

accordingly (cf B6)

$$G_{00}^{K} = -2i\pi V^2 \left|G_{00}^{r}(W)\right|^2 \left(\varrho_L^0(W)\,\mathcal{D}_L(W) + \varrho_R^0(W)\,\mathcal{D}_R(W)\right)$$

on the other hand, (cf B6B)

$$\Gamma(w) = i\pi \left(\rho_L^0(w) + \rho_R^0(w)\right) V^2$$

and

$$G_{00}^k = \left(G_{00}^r(w) - G_{00}^a(w)\right) \Delta_{AV}(w) \qquad \text{(B7A)}$$

with an "averaged" distribution function

$$\Delta_{AV}(w) = \frac{\rho_L^0(w)\Delta_L(w) + \rho_R^0(w)\Delta_R(w)}{\rho_L^0(w) + \rho_R^0(w)} \qquad \text{(B7A)}$$

which of course cannot be associated to any temperature and/or chemical potential

This is the first example of a nontrivial steady state

In this situation it is interesting to evaluate the current

Current

The current operator ^is defined via

$$\hat{I} = -d\frac{\hat{Q}}{dt}$$

for example, if I is the current flowing away from the L lead, then Q is its total charge

$$\hat{I}_L = -\frac{d\hat{Q}_L}{dt} = -e\sum_{p<0}\frac{d}{dt}c_p^+ c_p$$

$$= -e\sum_{p<0} i\left[H, c_p^+ c_p\right] = -ie\sum_{p<0} V_{p0}\left(d^+ c_p - c_p^+ d\right)$$

Its expectation value is evaluated with the Keldysh Green's function

$$\left\langle c_p^+ d\right\rangle = -\frac{i}{2}G_{0p}^K(t=0)$$

$$I_L = \left\langle \hat{I}_L\right\rangle = \frac{e}{2}\sum_{p<0} V_{p0}\left(G_{0p}^K(t=0) + c.c.\right)$$

$$= e\sum_{p<0} V_{p0}\,\mathrm{Re}\,G_{0p}^K(t=0) \qquad \text{(B8)}$$

Fourier transformation: $$G_{0p}^K(t=0) = \int\frac{dw}{2\pi}G_{0p}^K(w) \qquad \text{(B8A)}$$

and we now work in frequency space

with the help of Dyson's equation we get $$G_{0p} = G_{00}V_{0p}g_p$$

for the Keldysh component

$$G^K_{0\rho} = \left(G^r_{00}\, \vartheta^K_{\rho\rho} + G^K_{00}\, \vartheta^a_{\rho\rho} \right) V_{0\rho}$$

(cf. B7A)

$$\left(G^r_{00} \left(\vartheta^r_{\rho\rho} - \vartheta^a_{\rho\rho} \right) \delta_L(w) + \left(G^r_{00} - G^a_{00} \right) \delta_{AV}(w)\, \vartheta^a_{\rho\rho} \right) V_{0\rho}$$

In view of evaluating I, for constant V, we need the sum over p of this expression (cf B8 , B6A)

$$\sum_{\rho<0} \ldots = V \left(G^r_{00} \left(-2i\pi \varrho^0_L \right) \delta_L(w) + \left(G^r_{00} - G^a_{00} \right) \left(R_L + i\pi \varrho^0_L \right) \delta_{AV}(w) \right)$$

$$R_L = \mathrm{Re} \sum_{\rho<0} \vartheta^r_{\rho\rho} \qquad \text{and} \qquad \vartheta^a_{\rho\rho} = \vartheta^{r\,*}_{\rho\rho}$$

For the current one needs the real part of this. Since $\left(G^r_{00} - G^a_{00} \right)$ is imaginary we get (cf B8, B8A)

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

with

$$\eta(w) = \varrho^0_L \delta_L\, \mathrm{Im}\, G^r_{00} - \mathrm{Im}\, G^r_{00}\, \varrho^0_L \delta_{AV}$$

$$\left(\mathrm{Im}\, G^r_{00} \right) \varrho^0_L \left(\delta_L - \delta_{AV} \right)$$

$$\mathrm{Im}\, G^r_{00}(w) = -\pi A_{00}(w)$$

is the spectral function of the central region

which can also be written as (cf B6C)

$$-\pi V^2 \left| G^r_{00} \right|^2 \left(\varrho^0_L + \varrho^0_R \right)$$

(CF B7B)

$$\Delta_L - \Delta_{AV} = \frac{\Delta_L \rho_L^0 + \Delta_L \rho_R^0 - \rho_L^0 \Delta_L - \rho_R^0 \Delta_R}{\rho_L^0 + \rho_R^0}$$

$$= \frac{(\Delta_L - \Delta_R)\,\rho_R^0}{\rho_L^0 + \rho_R^0}$$

$$\Delta_L - \Delta_R = 2\left(n_R(w) - n_L(w)\right) \qquad \text{for fermions}$$

$$= 2\left(f_F(w-\mu_R) - f_F(w-\mu_L)\right)$$

$$\gamma(w) = 2\pi\, A_{00}(w)\, \frac{\rho_L^0 \rho_R^0}{\rho_L^0 + \rho_R^0}\left(f_F(w-\mu_L) - f_F(w-\mu_R)\right)$$

equivalently (Cf. B6C)

$$\gamma(w) = 2\pi V^2 |G_{00}^{\pi}|^2\, \rho_L^0 \rho_R^0 \left(f_F(w-\mu_L) - f_F(w-\mu_R)\right)$$

I.e., we can express the current as

$$I = e \int \frac{dw}{2\pi} \gamma(w)\, \rho_L^0(w)\, \rho_R^0(w) \left(f_F(w-\mu_L) - f_F(w-\mu_R) \right)$$

with

$$\gamma(w) = 4\pi^2 V^4 \left| G_{00}^r(w) \right|^2$$

remember

$$\left| G_{00}^r(w) \right|^2 = \frac{1}{\left(w - E(w)\right)^2 + \pi V^2 \left(\rho_L^0 + \rho_R^0\right)}$$

Which has a simple interpretation:
at each energy w electrons contribute in proportion to the combined density of states L and R and to the difference of occupations (Fermi function) between L and R multiplied

by an energy dependent transmission coefficient, $\gamma(w)$