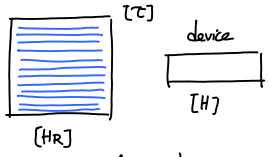
Session 12

Note Title 11/2/2008

Level broadening

The Hamiltonian for the entire system of the device and reservoir is: $\bar{H} = \begin{bmatrix} H & \tau \\ \tau^+ & H_R \end{bmatrix}$



where $[H]$ and $[H_R]$ are the Hamiltonian matrices for the device and reservoir separately and $[\tau]$ is the interaction part.

The spectral function for the entire system is: $\bar{A} = 2\pi\delta(EI - \bar{H})$ (this $-$ indicates entire system)

$$= i\left\{ [(E+i0^+)I - \bar{H}]^{-1} - [(E-i0^+)I - \bar{H}]^{-1} \right\}$$

$$= i[\bar{G} - \bar{G}^+]$$

$$= \begin{bmatrix} A & A_{dR} \\ A_{Rd} & A \end{bmatrix}$$

If we knew A in the device, we would be able to calculate other parameters like electron density or local density of states. We are interested only in the device part A. So we would like to find only A. For this we need to extract G from $\bar{G}$ matrix.

$$\bar{G} = [(E+i0^+)I - H]^{-1} = \begin{bmatrix} \overbrace{(E+i0^+)I - H}^{a} & -\tau \\ -\tau^+ & \underbrace{(E+i0^+)I - H_R}_{b} \end{bmatrix}^{-1} = \begin{bmatrix} G & G_{dR} \\ G_{Rd} & G_R \end{bmatrix} \Rightarrow \begin{bmatrix} a & -\tau \\ -\tau^+ & d \end{bmatrix}\begin{bmatrix} G & G_{dR} \\ G_{Rd} & G_R \end{bmatrix} = I \rightarrow \begin{cases} aG - \tau G_{dR} = I & aG - \tau d^{-1}\tau^+ G = 0 \\ -\tau^+ G + d G_{dR} = 0 & \rightarrow \end{cases}$$

$$G_{dR} = d^{-1}\tau^+ G$$

$$\rightarrow G = [a - \tau d^{-1}\tau^+]^{-1}$$

Self energy Σ

$$\vec{d} = [(E+i0^+)I - H_R]^{-1} = G_R \rightarrow$$

$$\boxed{G = [(E+i0^+)I - H - \Sigma]^{-1}}$$

$$\boxed{\Sigma = \tau G_R \tau^+}$$

Note that self-energy Σ has the same size as the device:

$\Sigma = \tau\ G_R\ \tau^+$

$d\times R\quad R\times R\quad R\times d \rightarrow d\times d$

So in order to calculate G, we need to find Σ first. But that seems to require calculating G_R which is a very large matrix (remember that reservoir is very large). So how can we find Σ? Well, fortunately τ and τ^+ in Σ are matrices with only one non-zero element (in 1D) at the device-reservoir boundary:

$$\tau = \begin{matrix} d \downarrow \\ \end{matrix} \overset{R \rightarrow}{\begin{bmatrix} -t_0 & 0 & \cdots \\ 0 & 0 & \\ \vdots & & \ddots \end{bmatrix}} = \tau^+ \Rightarrow \Sigma = \tau G_R \tau^+ = \begin{bmatrix} -t_0 & 0 & \cdots \\ 0 & 0 & \\ \vdots & & \ddots \end{bmatrix}\begin{bmatrix} G_R(0,0) & \cdots \\ \vdots & \ddots \end{bmatrix}\begin{bmatrix} -t_0 & 0 & \cdots \\ 0 & 0 & \\ \vdots & & \ddots \end{bmatrix} = \begin{bmatrix} t_0^2 G_R(0,0) & 0 & \cdots \\ 0 & 0 & \\ \vdots & & \ddots \end{bmatrix}$$

So Σ has only one non-zero element which is:

$$\boxed{\Sigma_{11} = t_0^2 G_R(0,0)}$$

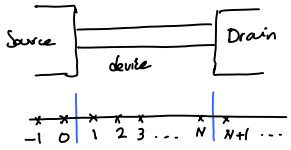
$G_R(0,0)$ is called Surface Green's function as it is calculated only at the surface boundary of the reservoir with the device.

What is $G_R(0,0)$?

For a one-dimentional effective mass approximation we have:

$$\text{Given } G_R = [(E+i0^+)I - H_R]^{-1} = \begin{bmatrix} E+i0^+ - E_c - 2t_0 & t_0 & & \\ t_0 & \ddots & \ddots & \\ & \ddots & \ddots & t_0 \\ & & t_0 & E+i0^+ - E_c - 2t_0 \end{bmatrix}^{-1} \Rightarrow G_R^{-1} G_R = I$$

$\leftarrow$ Tridiagonal



$$\left[G_R^{-1}\right]\left[G_R\right]^{0\ -1\ -2\ \cdots} = I \rightarrow$$

$$[(E+i0^+) - E_c - 2t_0]G_R(0,0) + t_0 G_R(-1,0) = 1 \quad (1)$$

$$t_0 G_R(0,0) + [(E+i0^+) - E_c - 2t_0]G_R(-1,0) + t_0 G_R(-2,0) = 0 \quad (2)$$

$$\vdots$$

$G_R(0,0)e^{ika}$, $G_R(0,0)e^{ika}$, $G_R(0,0)e^{i2ka}$

Because this is periodic, we may apply the ansatz: $G_R(n,0) = G_R(0,0)e^{-inka}$

(2) $\rightarrow$ $t_0 e^{-ika} + (E+i0^+) - E_c - 2t_0 + t_0 e^{ika} = 0 \rightarrow (E+i0^+) = E_c + 2t_0(1-\cos ka)$

(1) $\rightarrow$ $G_R(0,0) = \dfrac{1}{(E+i0^+) - E_c - 2t_0 + t_0 e^{ika}}$ Substitute $E+i0^+$ to get :

$$\boxed{G_R(0,0) = -\frac{1}{t_0}e^{ika}}$$

$\Sigma_{11} = t_0^2 G_R(0,0) \Rightarrow$ $\boxed{\Sigma_{11} = -t_0 e^{ika}}$ From Σ we can calculate, G, A, and finally ρ.

Note: A very important property of the self-energy matrix Σ is that it is anti-Hermitian, i.e: $\Sigma^\dagger = -\Sigma$

Also notice that Σ depends on k which itself depends on energy, i.e $\Sigma(E)$.

Physical meaning of the Green's function

It is easier to consider the eigenstate space representation of G:

$$G = \left[(E+i0^+)I - H\right]^{-1} = \left[(E+i0^+)I - VDV^\dagger\right]^{-1} = V\underbrace{\left[(E+i0^+)I - D\right]^{-1}}_{G(E)\text{ in eigenstate space}}V^\dagger$$

(G in real space)

note: $D = \begin{bmatrix} \varepsilon_1 & & 0 \\ & \varepsilon_2 & \\ 0 & & \ddots \end{bmatrix}$

$G(E)$ is now diagonal (because D is diagonal): $G(E) = \begin{bmatrix} \frac{1}{E-\varepsilon_1+i0^+} & 0 & \cdots \\ 0 & \frac{1}{E-\varepsilon_2+i0^+} & \\ \vdots & & \ddots \end{bmatrix}$. If we now fourier transform $G(E)$, we will have the G in time domain (remember energy and time domains are fourier transformed to each other):

$$\tilde{G}(t) = \frac{1}{2\pi}\int d\omega\, G(\omega)e^{-i\omega t} = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dE}{\hbar}G(E)e^{-i\frac{E}{\hbar}t} \qquad \text{note: } E=\hbar\omega.$$

To make it simple, let's consider a one energy level device, ε_1. So $G(E)$ is 1x1 and equal to $\frac{1}{E-\varepsilon_1+i0^+}$:

$$\tilde{G}(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dE}{\hbar}\frac{1}{E-\varepsilon_1+i0^+}e^{-i\frac{E}{\hbar}t} = -\frac{i}{\hbar}\theta(t)e^{-i\frac{\varepsilon_1}{\hbar}t}e^{-0^+t} \qquad (\theta \text{ is the step function})$$

To see how this works, let's do the inverse Fourier Transform:

$$G(E) = \int_{-\infty}^{\infty}dt\,\tilde{G}(t)e^{i\frac{E}{\hbar}t} = \frac{-i}{\hbar}\int_0^{\infty}dt\,e^{-i\frac{\varepsilon_1}{\hbar}t}e^{i\frac{E}{\hbar}t}e^{-0^+t} = -\frac{i}{\hbar}\left[\frac{e^{i(E-\varepsilon_1)t/\hbar}e^{-0^+t}}{\left[i(E-\varepsilon_1)-0^+\right]/\hbar}\right]_0^{\infty}$$

$$= \frac{i}{\hbar}\frac{1}{\left[i(E-\varepsilon_1)-0^+\right]/\hbar} = \frac{1}{E-\varepsilon_1+i0^+}$$

So $\tilde{G}(t) = -\frac{i}{\hbar}\theta(t)e^{-i\frac{\varepsilon_1}{\hbar}t}e^{-0^+t}$ is the time domain version of $G(E)$.

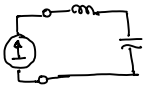
we can check that $\tilde{G}(t)$ satisfies the following Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\tilde{G}(t) - (\varepsilon_1 - i0^+)\tilde{G}(t) = \delta(t)$$

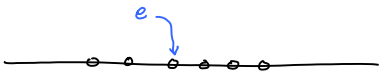
It means that we can physically look at the Green's function as the Impulse Response of the Schrödinger equation:

$\left(i\hbar\frac{\partial}{\partial t} - H + i0^{+}I\right)\tilde{G}(t) = \delta(t)\,I$ of the general Schrödinger equation: $\left(i\hbar\frac{\partial}{\partial t} - H\right)\Psi(t) = 0$

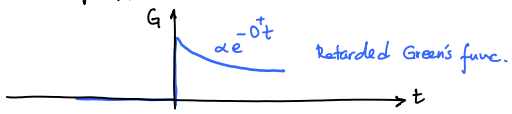
In general, we can look at the impulse response of any differential equation. For example, for the Porsson's equ:

$\nabla^2\Phi = -\frac{\rho}{\varepsilon} \longrightarrow \nabla^2 G = -\delta(t)$ or for an LC circuit: $V=\delta(t)$  , etc.

Another example is that an impulse excitation of the Schrödinger equation in 1D might be viewed as injecting one electron into a nanowire:



Also, notice that $+i0^{+}$ in G and $-i0^{+}$ in G^{+} results in two worlds of opposite in time domain:

$G(t) = \frac{-i}{\hbar}\theta(t)\,e^{-i\frac{\varepsilon}{\hbar}t}\,e^{-0^{+}t} \longrightarrow$ 

$G^{+}(t) = \frac{i}{\hbar}\theta(-t)\,e^{-i\frac{\varepsilon}{\hbar}t}\,e^{0^{+}t} \longrightarrow$ 

Physical meaning of the Self-energy Σ

Recall that for the device region we had: $G = [EI - H - \Sigma]^{-1} \rightarrow [EI - H - \Sigma]G = I$

We can translate this similarly in time domain as: $\left(i\hbar\frac{\partial}{\partial t} - H - \Sigma\right)G(t) = I\,\delta(t)$

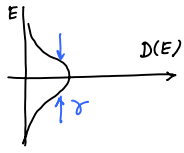
For simplicity let's again consider a single energy level device: $\left(i\hbar\frac{\partial}{\partial t} - \varepsilon - \Sigma\right)G(t) = \delta(t) \rightarrow G(t) = e^{-i\frac{\varepsilon}{\hbar}t}\,e^{-i\frac{\Sigma}{\hbar}t}\,\theta(t)$

Σ is complex in general (recall for a 1D device we had $\Sigma = -t_0 e^{ika}$): $\Sigma = \mathrm{Re}(\Sigma) + i\,\mathrm{Im}(\Sigma) \rightarrow$

$$G = e^{-i\frac{\varepsilon'}{\hbar}t}\,e^{-i\frac{\gamma}{2\hbar}t}\,\theta(t) \quad \text{where we defined: } \varepsilon' \equiv \varepsilon + \mathrm{Re}(\Sigma) \text{ and } \gamma \equiv -2\,\mathrm{Im}(\Sigma)$$

Therefore, physically the real part of self energy Σ makes an energy shift in the device, and its imaginary part (times −2) is the rate that electron escapes from the device. The electron life time is define as:

$$\frac{1}{\tau} = \frac{\gamma}{\hbar} = \frac{-2\,\mathrm{Im}(\Sigma)}{\hbar} \rightarrow G(t) = \theta(t)\,e^{i\frac{\varepsilon'}{\hbar}t}\,e^{-t/2\tau}$$

γ is also related to the broadening of a level: 

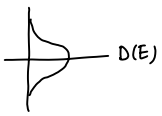
such that there is a uncertainty relation between lifetime and broadening: $\gamma\tau = \hbar$

To show how γ is related to broadening of a, let's calculated the density of states:

Note: In general $D(E) = \frac{1}{2\pi}\,\mathrm{Trace}[A(E)]$

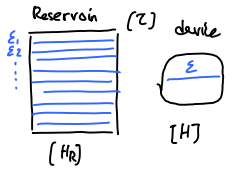
$A(E) = i(G - G^{+})$ for 1 level device $G(E) = \frac{1}{E - \varepsilon' + \frac{i\gamma}{2}} \rightarrow D(E) = \frac{A(E)}{2\pi} = \frac{i}{2\pi}\left(\frac{1}{E - \varepsilon' + \frac{i\gamma}{2}} - \frac{1}{E - \varepsilon' - \frac{i\gamma}{2}}\right)$

$\Rightarrow D(E) = \frac{\gamma/2\pi}{(E-\varepsilon')^2 + \left(\frac{\gamma}{2}\right)^2}$ This is exactly the 1-level device DOS Lorentzian broadening that we discussed at the beginning of the course!



So the level broadening and lifetime are both described by imaginary part of the self-energy Σ.

Physical meaning of $i0^+$



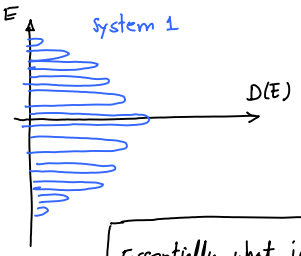
If the device and the reservoir are decoupled, in the eigenstate space we have:

$$\frac{A(E)}{2\pi} = \begin{bmatrix} \delta(E-\mathcal{E}) & & 0 \\ & \delta(E-\mathcal{E}_1) & \\ 0 & & \delta(E-\mathcal{E}_2) \\ & & \ddots \end{bmatrix}$$

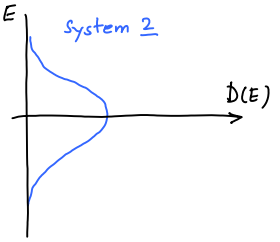
Similarly, when they are coupled, the overal Hamiltonian is: $H = \begin{bmatrix} \mathcal{E} & \tau_1 & \tau_2 & \cdots \\ \tau_1^+ & \mathcal{E}_1 & & \\ \tau_2^+ & & \mathcal{E}_2 & \ddots \\ \vdots & & & \end{bmatrix}$

With wavefunctions leaking out from both sides of the device, the resulting LDOS on the device may look like either of:

LDOS for small coupling:



LDOS for full coupling:

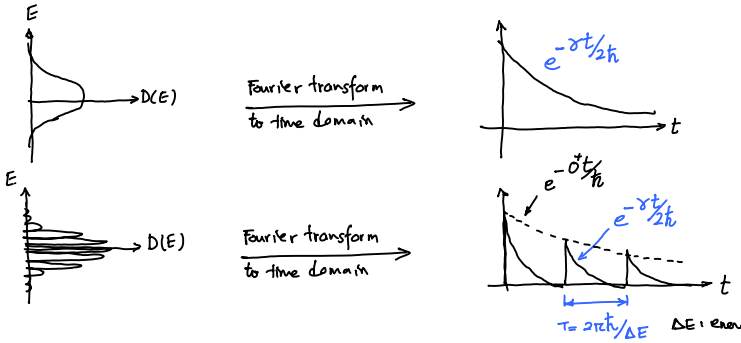


Essentially what $i0^+$ term does is broaden out these spikes into a continous DOS.

So what is the physical difference between system 1 and system 2? this difference is best described illustrated in time domain.

The spiked DOS represents a reversible repeating system (or an electron oscillating back and forth between the device and reservoir) with a period of $T = \frac{2\pi\hbar}{\Delta E}$.

The continous DOS represents a non-reversible DOS where an electron escapes the device and never comes back.

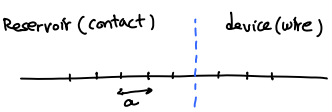


ΔE: energy spacing in the reservoir.

So $i0^+$ adds an irreversibility decay in the time domain, preventing the electron from oscillating back and forth from the reservoir. This is how it broadens the DOS. It acts as a dampening factor and thereby enables us to model the irreversible physical nature of most infinite systems with finite sized numerical models. So to get the broadened DOS, 0^+ must be larger than ΔE. In large reservoirs, ΔE is very small or often Σ is large enough that the broadening of the peaks is already taken care of:

$$0^+ > \Delta E \text{ or in large reservoirs } \Sigma\uparrow \text{ and } \Delta E\downarrow \Rightarrow \text{Broadened DOS (system 2)}$$

Example: Calculate the electron velocity in a 1-D lattice and show that the electron lifetime corresponds to $\frac{1}{\tau} = \frac{\gamma}{\hbar}$.



We know for this lattice: $E = E_c + 2t_o(1-\cos ka)$. The state velocity is given by:

$$v = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \frac{2at_o \sin ka}{\hbar} \rightarrow \frac{1}{\tau} = \frac{v}{a} = \frac{2t_o \sin ka}{\hbar} \quad (1)$$

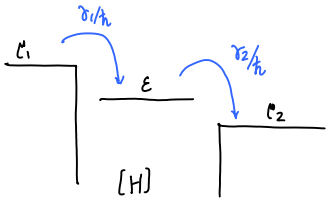
We also have: $\Sigma = \tau G_R \tau^+ = t_o\left(-\frac{e^{ika}}{t_o}\right)t_o = -t_o e^{ika} \rightarrow \mathrm{Im}(\Sigma) = -t_o \sin ka = -\frac{\gamma}{2}$

$\rightarrow t_o \sin ka = \frac{\gamma}{2}$ Substitute in (1) $\Rightarrow \frac{1}{\tau} = \frac{\gamma}{\hbar}$ and $v = \frac{a\gamma}{\hbar}$

This gives a relation between the self-energy and the electron escape velocity from a reservoir coupling unit cell into the device.

Non-equilibrium transport

We now return to the problem of current flow through our device. We saw before that current in a FET is given by:



$I = \frac{2e}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}(f_1-f_2)$ or considering the broadening: $I = \frac{2e}{\hbar}\int dE\, D(E)\underbrace{\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}}_{\equiv T(E)/2\pi}(f_1-f_2)$

$T(E)$ is the transmission function.

In matrix form the imaginary part of Σ can be written as $\Gamma = i(\Sigma - \Sigma^\dagger) \quad = -2\,\mathrm{Im}(\Sigma)$

Note that: $\Sigma = \mathrm{Re}(\Sigma) + i\,\mathrm{Im}(\Sigma) \rightarrow \Sigma - \Sigma^\dagger = \mathrm{Re}(\Sigma) + i\,\mathrm{Im}(\Sigma) - (\mathrm{Re}(\Sigma) - i\,\mathrm{Im}(\Sigma)) = 2i\,\mathrm{Im}(\Sigma)$

γ_1 and γ_2 are also not constants in general and follow from Σ_1 and Σ_2: $\Gamma_1 = i(\Sigma_1 - \Sigma_1^\dagger)$, $\Gamma_2 = i(\Sigma_2 - \Sigma_2^\dagger)$.

$\Gamma_{1,2}$ are responsible for broadening. They are energy dependent.

We can also write: $\Sigma_{1,2} = \frac{\Sigma_{1,2}+\Sigma_{1,2}^\dagger}{2} + \frac{\Sigma_{1,2}-\Sigma_{1,2}^\dagger}{2} = \frac{\Sigma_{1,2}+\Sigma_{1,2}^\dagger}{2} - \frac{i\Gamma_{1,2}}{2}$

For our FET device, the total self-energy is $\Sigma = \Sigma_1 + \Sigma_2 \rightarrow G = (EI - H - \Sigma)^{-1}$

Having the Green's function, we can calculate all other quantities such as the spectral function A: $A = i(G - G^\dagger)$.

For the total number of electrons N in the channel we had: $N = \frac{\gamma_1 N_1 + \gamma_2 N_2}{\gamma_1+\gamma_2} = \frac{1}{\gamma_1+\gamma_2}\int dE\,(\gamma_1 D(E) f_1 + \gamma_2 D(E) f_2)$

In matrix form we have: $N = \mathrm{Trace}\int dE\,\underbrace{(A_1 f_1 + A_2 f_2)}_{G^n}$ where: $A_1 = G\Gamma_1 G^\dagger$; $A_2 = G\Gamma_2 G^\dagger$

matrix is: $T(E) = \mathrm{Trace}\,(\Gamma_1 G \Gamma_2 G^\dagger)$

Transmission: $A = A_1 + A_2$ and $A_1 f_1 + A_2 f_2 = G^n$

For the current at the source and drain we had: $I_{1,2} = -\frac{e}{\hbar}\int dE\,\gamma_{1,2}\,(D(E) f_1 - n(E))$

we now have: $I_i = -\frac{e}{\hbar}\int dE\,[\mathrm{Trace}(\Gamma_i A) f_i - \mathrm{Trace}(\Gamma_i G^n)]$

And the net current is: $I = -\frac{e}{\hbar}\,dE\,\underbrace{\mathrm{Trace}\,(\Gamma_1 G \Gamma_2 G^\dagger)}_{T(E)}(f_1 - f_2)$

Summary of results:

$G = (EI - H - \Sigma)^{-1}$; $\Sigma = \Sigma_1 + \Sigma_2$

$\Gamma_1 = i(\Sigma_1 - \Sigma_1^\dagger)$; $\Gamma_2 = i(\Sigma_2 - \Sigma_2^\dagger)$; $\Gamma = i(\Sigma - \Sigma^\dagger)$

$A_1 = G\Gamma_1 G^\dagger$; $A_2 = G\Gamma_2 G^\dagger$

$A = i(G - G^\dagger) = A_1 + A_2$

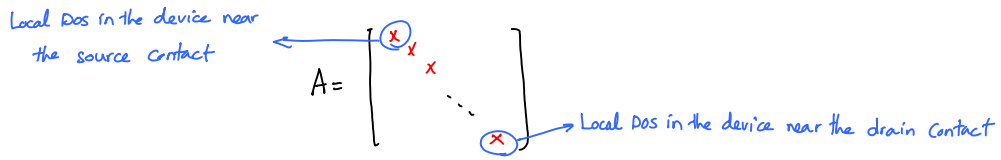
$T(E) = \mathrm{Trace}\,(\Gamma_1 G \Gamma_2 G^\dagger)$

$G^n = A_1 f_1 + A_2 f_2$

$I_i = -\frac{e}{\hbar}\int dE\,[\mathrm{Trace}\,(\Gamma_i A_i) f_i - \mathrm{Trace}\,(\Gamma_i G^n)]$

$I = -\frac{e}{\hbar}\int dE\,T(E)(f_1 - f_2)$

Note on A_1 and A_2: When the device is connected to two reservoirs (source and drain), the DOS can be broken into 2 parts corresponding to A_1 and A_2. Then $A = A_1 + A_2$. Here A_1 gets filled according fermi function f_1 and A_2 gets filled according to f_2.



Note on G^n: G^n is electron density and tells us what's filled. It is calculated by summing $A_1 f_1$ with $A_2 f_2$.

Note on I: These equations are applicable to any type of complex problem to get the current passing through the device.

Example: Show that $T(E)$ in the limiting case of 1×1 matrix becomes what we had for the one level device.

$$H \to [\varepsilon]$$

$$\left.\begin{aligned}\Sigma_1 &\to \sigma_1 - \frac{i\gamma_1}{2}\\ \Sigma_2 &\to \sigma_2 - \frac{i\gamma_2}{2}\end{aligned}\right\} \Sigma = \Sigma_1 + \Sigma_2 = \overbrace{(\sigma_1+\sigma_2)}^{\sigma} - \frac{i}{2}\overbrace{(\gamma_1+\gamma_2)}^{\gamma} \to G = (EI - H - \Sigma)^{-1} = \frac{1}{E - \varepsilon - \sigma + \frac{i\gamma}{2}}$$

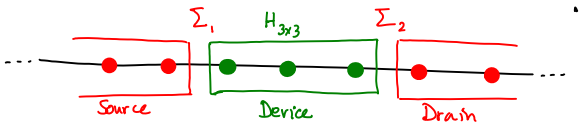
As for A_1 and A_2, we have: $A_i = G\gamma_i G^\dagger = \dfrac{\gamma_i}{(E-\varepsilon-\sigma)^2 + (\frac{\gamma}{2})^2} \to A = A_1 + A_2 = \dfrac{\gamma}{(E-\varepsilon-\sigma)^2 + (\frac{\gamma}{2})^2}$

Finally $T(E) = \gamma_1 G \gamma_2 G^\dagger = \dfrac{\gamma_1\gamma_2}{(E-\varepsilon-\sigma)^2 + (\gamma/2)^2}$ which similar to 1D case $T(E) = \underbrace{\dfrac{\gamma/2\pi}{(E-\varepsilon)^2 + (\frac{\gamma}{2})^2}}_{\text{Lorentzian DOS}} \times \dfrac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}$

Some notes on H and Σ

* H and Σ cannot by diagonalized simultaneously. So in eigenstate space where H is diagonal, Σ is not.

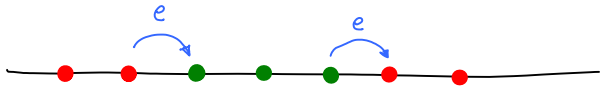
For example consider a three level device:



Real space representation of Σ and H:

$$\Sigma_1 = \begin{bmatrix} -t_0 e^{ika} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}; \quad H = \begin{bmatrix} E_C + 2t_0 + U_1 & t_0 & 0 \\ t_0 & E_C + 2t_0 + U_2 & t_0 \\ 0 & t_0 & E_C + 2t_0 + U_3 \end{bmatrix}; \quad \Sigma_2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -t_0 e^{ika} \end{bmatrix}$$

It shows electron transport in real space:



If we take H and $\Sigma_{1,2}$ into eigenstate space, H becomes diagonal $H = \begin{bmatrix} \varepsilon_1 & 0 & \\ 0 & \varepsilon_2 & \\ & & \varepsilon_3 \end{bmatrix}$; however, Σ_1 and Σ_2 will not be diagonal. In this space, the picture shows that an incoming electron will not just go into one level in the device, but it will go to all three energy levels in fractions. It is similar when the electron exits the device.

It will exit from all three levels. This is effected by the fact that Σ_1 and Σ_2 are not diagonal and have off diagonal terms: