Izmir: 10.08.09 - Lecture 2

CRANN

Quantitative theory for electron transport in nano-devices

Ivan Rungger
Computational Spintronics Group
School of Physics and CRANN, Trinity College Dublin

Trinity College The University of Dublin

sfi science foundation ireland

NDP NATIONAL DEVELOPMENT PLAN

SEVENTH FRAMEWORK PROGRAMME

HEA Higher Education Authority An tÚdarás um Ard-Oideachas

ENTERPRISE IRELAND

Main concepts of transport theory

- Green's functions, self-energies, gamma matrices
- **Current versus voltage (I-V) characteristics**
- **Transmission coefficient, density of states**
- Bias window
- Open vs. closed channels
- Strength of coupling, broadening of molecular levels
- Symmetry of coupling strength
- Movement of molecular levels with **charging**
- Potential drop and charging
- Level alignment

Green's functions

Green's functions vs. wave functions

$$G(E)=[(E+i\delta)S-H]^{-1}$$

$$\downarrow$$

$$G(E)=\sum_n \frac{1}{E+i\delta-\epsilon_n}\psi_n\psi_n^\dagger$$

Spectral function *A*: generalized density of states

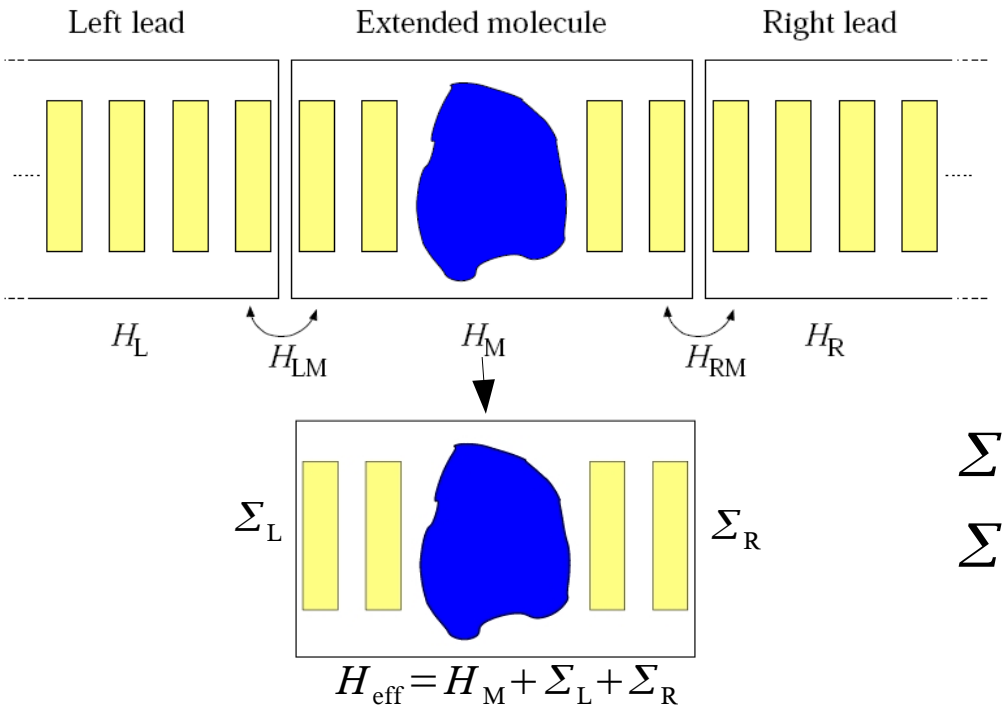
$$A(E)=i[G(E)-G^\dagger(E)] \longrightarrow \mathrm{DOS}(E)=\frac{1}{2\pi}\mathrm{Tr}[A(E)S]$$

Density matrix

$$\rho=\sum_n f(\epsilon_n)\,\psi_n\psi_n^\dagger \longrightarrow \rho=\frac{1}{2\pi}\int dE\; f(E)\;A(E)$$

The density matrix can equivalently be expressed in terms of wave functions and Green's functions

Non equilibrium Green's functions formalism



Σ_L : left self-energy

Σ_R : right self-energy

$$G(E) = [(E + i\delta) S_M - H_{eff}]^{-1}$$

$$\mu_L = \epsilon_F + \frac{eV}{2}$$

$$\mu_R = \epsilon_F - \frac{eV}{2}$$

Allows the calculation of the charge density at an applied bias potential.

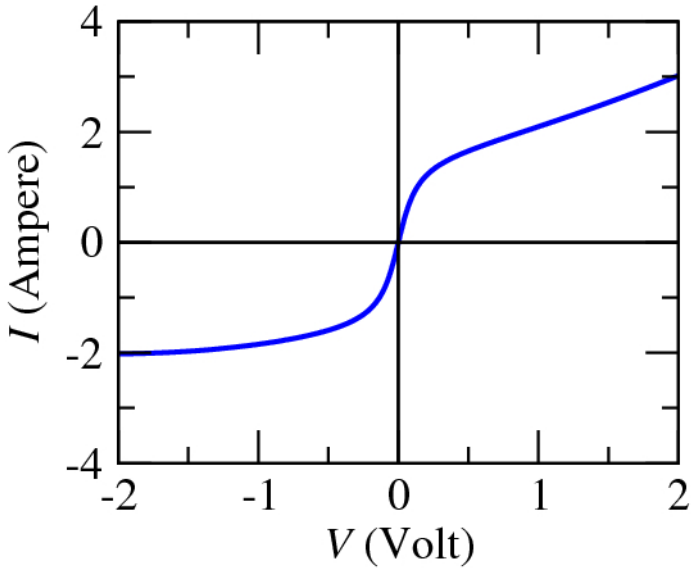
Coupling matrices (Γ-matrices)

$$\Gamma_{\mathrm{L}} = i\left(\Sigma_{\mathrm{L}} - \Sigma_{\mathrm{L}}^{\dagger}\right)$$

$$\Gamma_{\mathrm{R}} = i\left(\Sigma_{\mathrm{R}} - \Sigma_{\mathrm{R}}^{\dagger}\right)$$

- Gamma matrices: anti-Hermitian part of the self-energies.
- They introduce broadening of the molecular levels.
- They are a measure for the strength of the coupling of a level to the leads, and are therefore also called the coupling matrices.

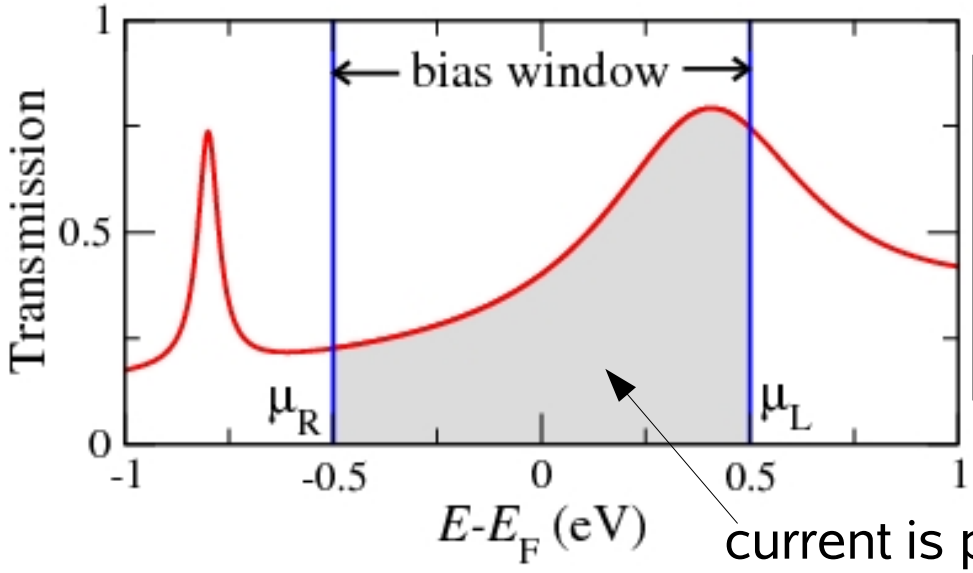
Current versus voltage (I-V)



- The I-V is what is measured in experiment
- Current can be different for positive and negative bias, it depends on the symmetry of the system

How do we calculate the current?

The current is obtained by integrating the transmission coefficient T over the bias window:



$$I(V)=\frac{e}{h}\int_{\mu_R}^{\mu_L} dE\ T(E,V)$$

$$T(E,V)=\mathrm{Tr}(\Gamma_L G^{\dagger}\Gamma_R G)$$

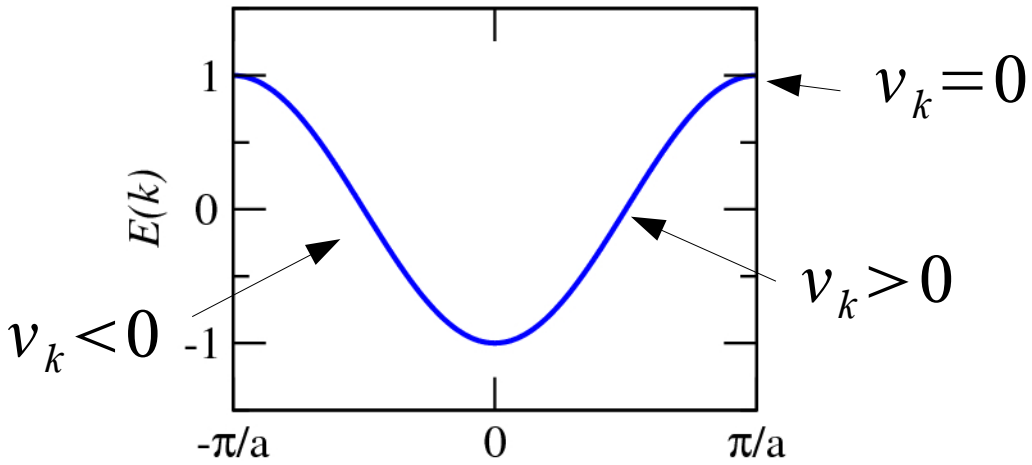
current is proportional to shaded area

- Bias window: The energy range between the left and right chemical potentials
- The current is proportional to the integral of the transmission coefficient over the bias window

Current of a Bloch state

In a periodic system each Bloch state carries a current proportional to its group velocity:

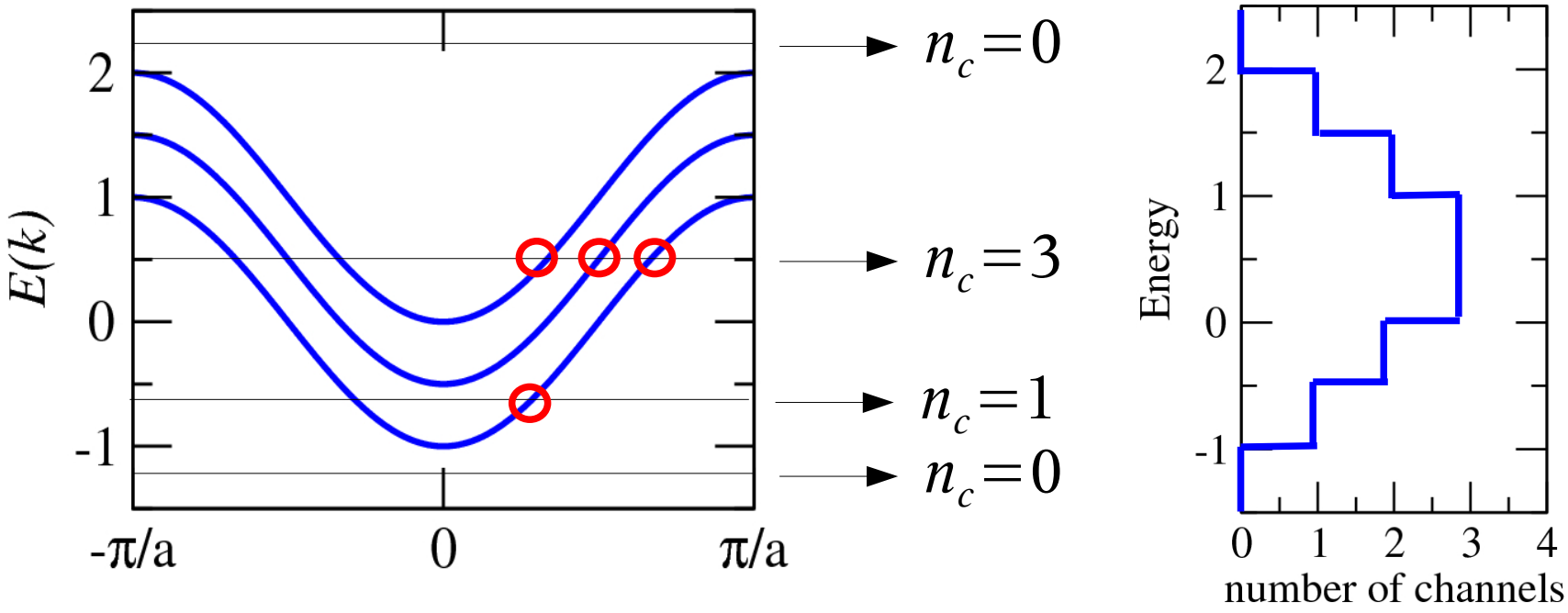
$$I_k \propto v_k \qquad v_k = \frac{1}{\hbar}\frac{\partial E(k)}{\partial k}$$



- At each energy the number of bands with positive group velocity is equal to the one with negative group velocity

- Number of channels: number of bands at a given energy with positive group velocity

Number of channels



- In the NEGF formalism all the information about the number of channels in the leads and their nature is contained in the self-energies.

Total current of periodic systems

To obtain the total current we need to consider the density of states:

$$\mathrm{DOS}_k = \frac{1}{\pi v_k}$$

The total current then is:

$$I(V) \propto \int_{\mu_L}^{\mu_R} dE \ \mathrm{DOS}_k I_k \propto \int_{\mu_L}^{\mu_R} dE \ \frac{1}{v_k} v_k = \int_{\mu_L}^{\mu_R} dE \ 1 = \mu_L - \mu_R$$

$$\downarrow$$

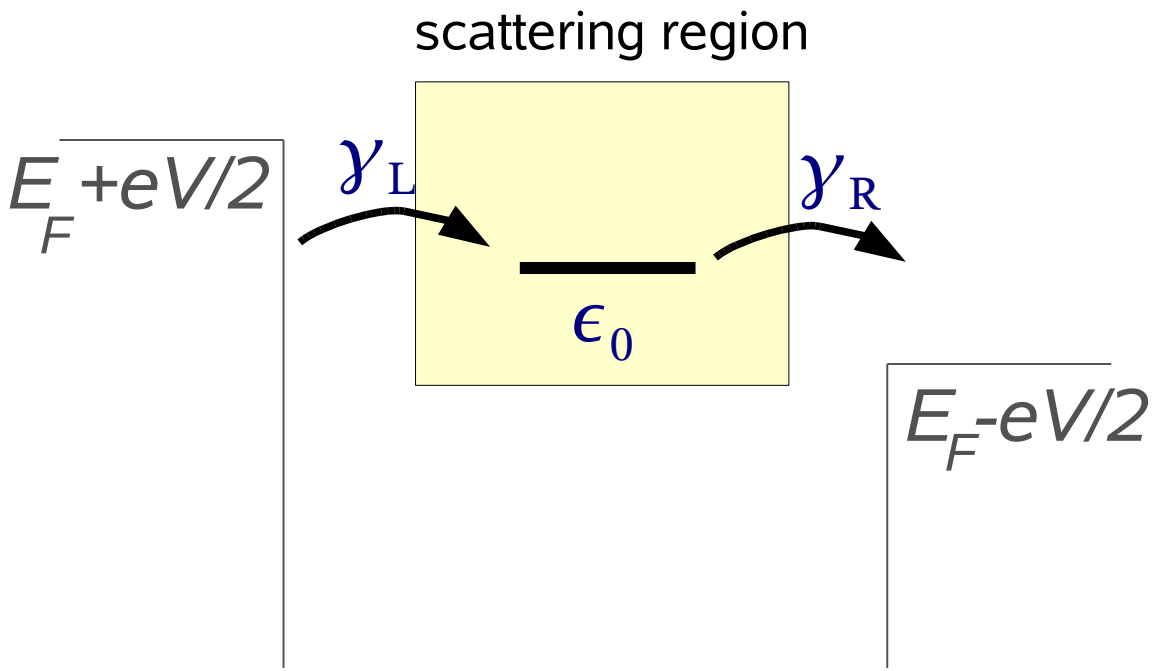
$$T_{\text{Bloch state}} = 1$$

- In a perfectly periodic system the transmission for a Bloch state is equal to one

- **Number of channels in the electrodes at a given energy sets the maximum transmission one can have at that energy**

Single level transport

Single level transport



- We use this simple analytical model to illustrate the next concepts
- The scattering region consists of a single molecular orbital
- For many levels the properties can be seen approximately as the superposition of single levels

Green's function

Green's function for the scattering region is given by:

$$G(E)=[E-H_{\text{eff}}]^{-1} \qquad H_{\text{eff}}=H_{\text{M}}+\Sigma_{\text{L}}(E)+\Sigma_{\text{R}}(E)$$

For this system we have:

$$H_{\text{M}}=\epsilon_0$$

We assume that the self-energies are constant for all energies:

$$\Sigma_{\text{L}}=\Sigma_{\text{R}}=-i\frac{\gamma}{2}$$

$$\Gamma_{\text{L}}=\Gamma_{\text{R}}=\gamma$$

- We therefore have two parameters: ϵ_0 and γ

The Green's function for this system therefore becomes:

$$G(E)=\frac{1}{E-\epsilon_0+i\gamma}$$

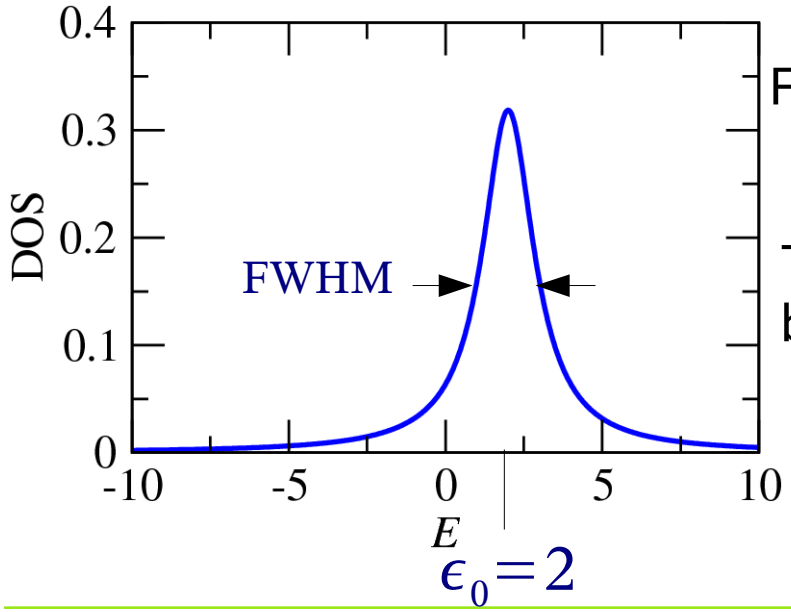
Density of states

The Green's function:

$$G(E)=\frac{1}{E-\epsilon_0+i\gamma}$$

Density of states:

$$\mathrm{DOS}(E)=\frac{i}{2\pi}[G(E)-G^{\dagger}(E)]=\frac{1}{\pi}\frac{\gamma}{(E-\epsilon_0)^2+\gamma^2}$$



Full width at half maximum (FWHM):

$$\mathrm{FWHM}=2\gamma$$

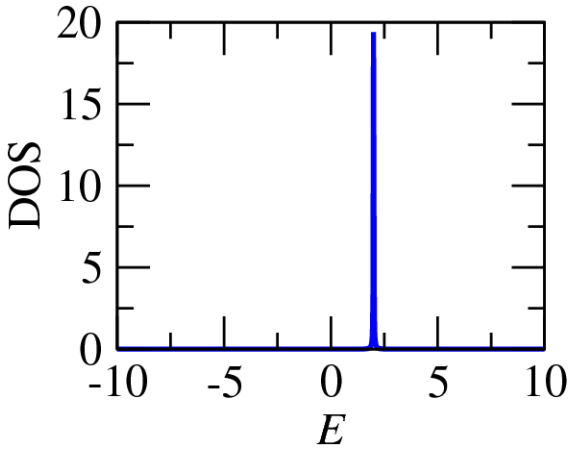
The coupling Gamma-matrices lead to a broadening of the molecular level.

Number of states:

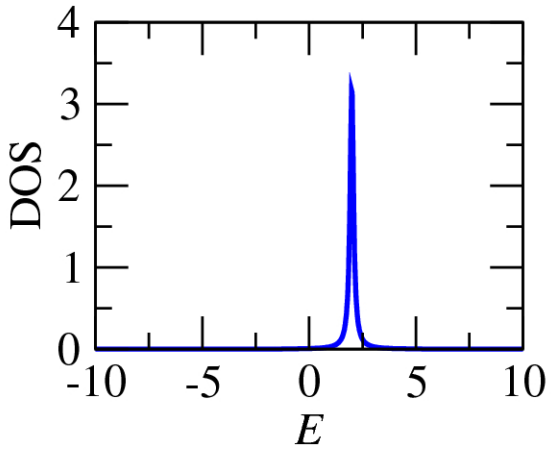
$$\int dE\,\mathrm{DOS}(E)=1$$

Weak and strong coupling

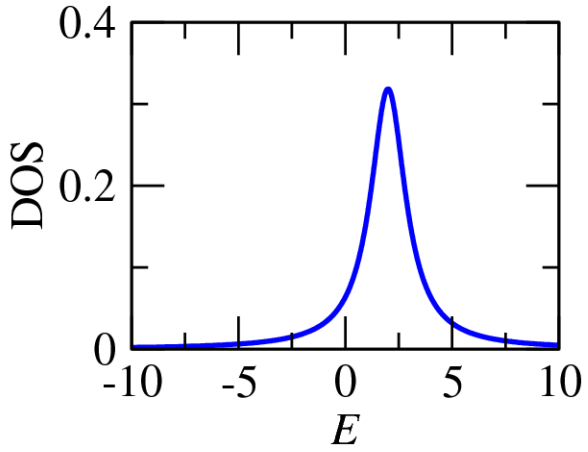
$$\mathrm{DOS}(E)=\frac{1}{\pi}\frac{\gamma}{(E-\epsilon_0)^2+\gamma^2}$$



weak coupling



intermediate coupling



strong coupling

NEGF+DFT approximation is better for stronger coupling

Transmission versus DOS

Transmission coefficient:

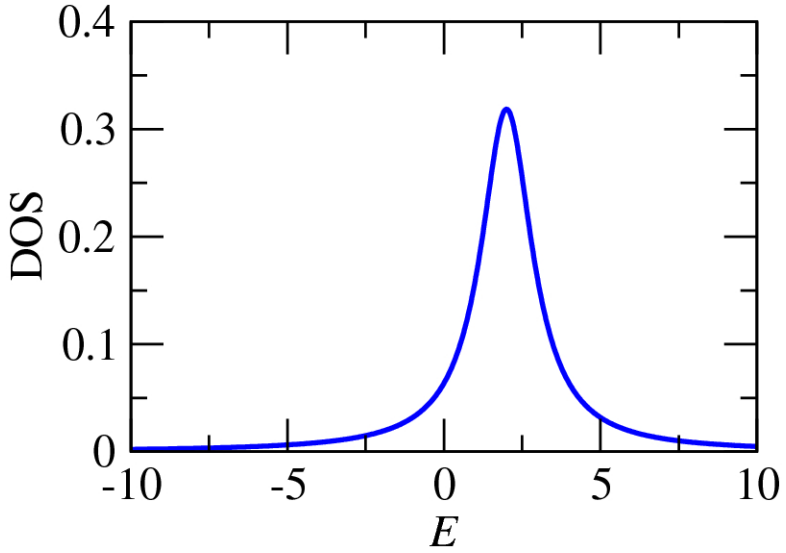
$$T(E,V)=\mathrm{Tr}(\Gamma_{\mathrm{L}}G^{\dagger}\Gamma_{\mathrm{R}}G)=\gamma\frac{1}{E-\epsilon_0+i\gamma}\gamma\frac{1}{E-\epsilon_0-i\gamma}$$

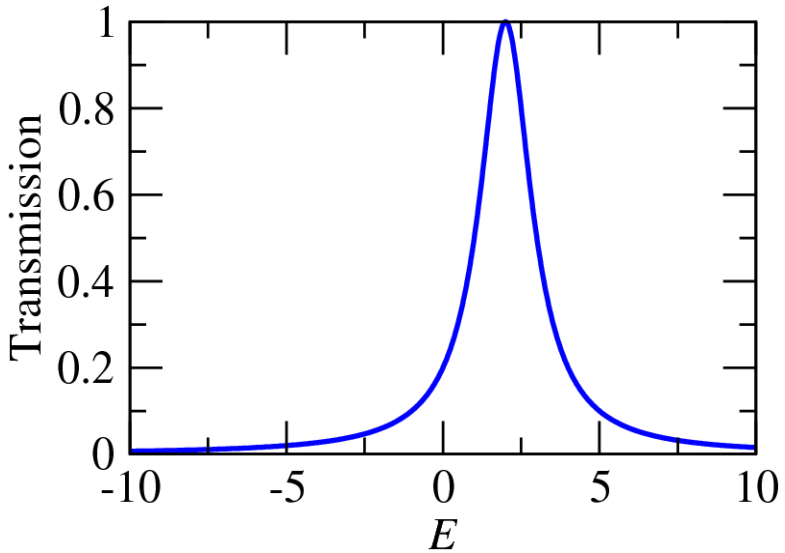
$$T(E)=\frac{\gamma^2}{(E-\epsilon_0)^2+\gamma^2}$$

Transmission versus DOS

$$\mathrm{DOS}(E)=\frac{1}{\pi}\frac{\gamma}{(E-\epsilon_0)^2+\gamma^2}$$

$$T(E)=\frac{\gamma^2}{(E-\epsilon_0)^2+\gamma^2}$$





- The transmission coefficient has a maximum at the same place where the DOS has a maximum, and is small where the DOS is small, and also the FWHM is equal

- Generally therefore **a peak in the DOS leads to a peak in the transmission**

Asymmetric coupling

- Until now we have assumed that left and right self-energies are identical. What if they are different?

$$\Sigma_L = -i\frac{\gamma_L}{2} \qquad \Sigma_R = -i\frac{\gamma_R}{2}$$
$$\Gamma_L = \gamma_L \qquad \Gamma_R = \gamma_R$$

- In this case DOS and transmission become:

$$\mathrm{DOS}(E) = \frac{1}{2\pi}\frac{\gamma_L+\gamma_R}{(E-\epsilon_0)^2+\frac{(\gamma_L+\gamma_R)^2}{4}}$$

$$T(E) = \frac{\gamma_L\gamma_R}{(E-\epsilon_0)^2+\frac{(\gamma_L+\gamma_R)^2}{4}}$$

$$T(E) = 2\pi\,\mathrm{DOS}(E)\frac{\gamma_L\gamma_R}{\gamma_L+\gamma_R}$$

Asymmetric coupling

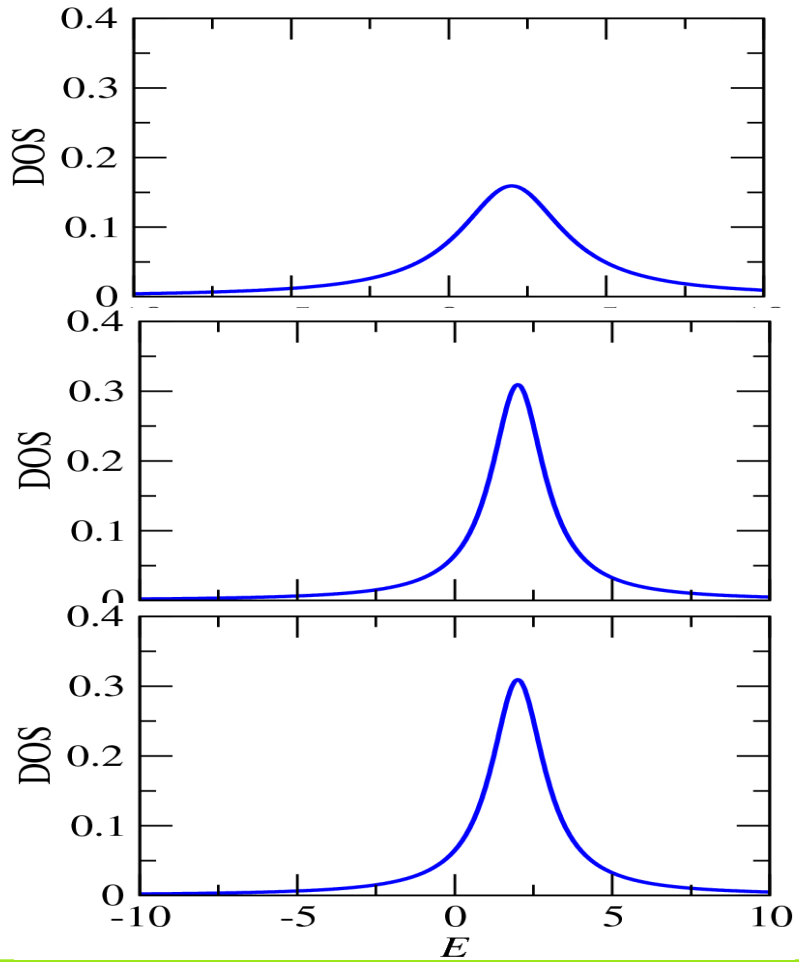
$$\mathrm{DOS}(E)$$

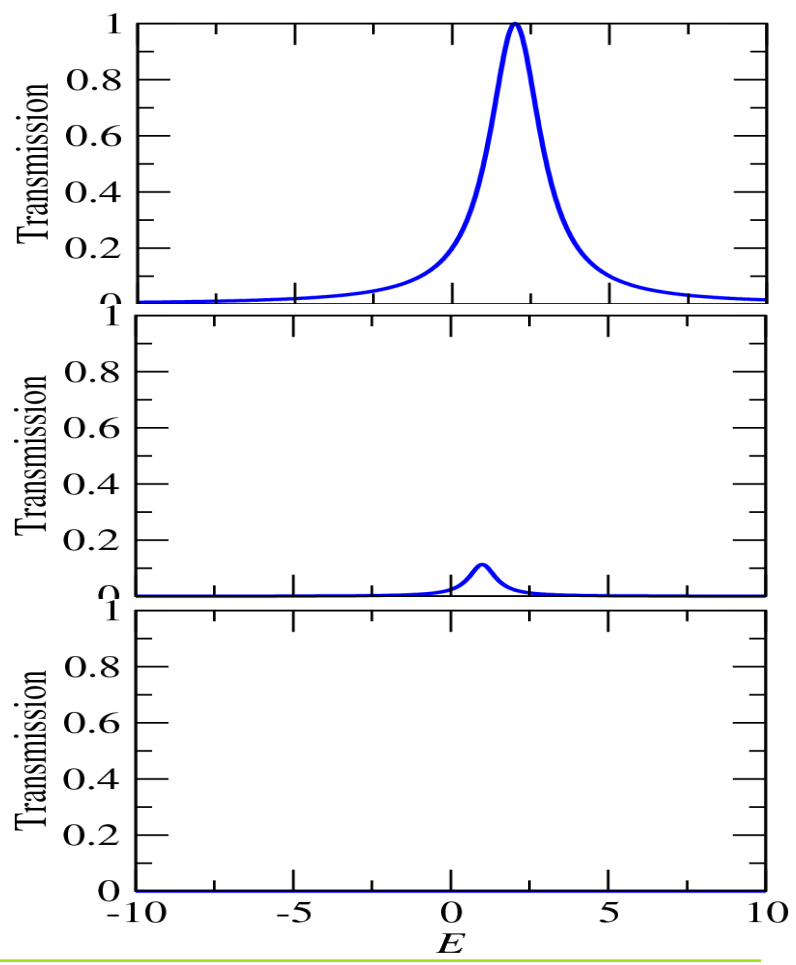
$$T(E)=2\pi\,\mathrm{DOS}(E)\frac{\gamma_L\gamma_R}{\gamma_L+\gamma_R}$$

$\gamma_L=\gamma_R$

$\gamma_L\gg\gamma_R$

$\gamma_R=0$





Asymmetric coupling

- The **DOS and broadening are not strongly affected by asymmetry** of the coupling
- The **transmission on the other hand is strongly affected by asymmetry:** the height of the transmission peak is maximal for equal coupling, and decreases as the coupling becomes asymmetric. It becomes exactly zero if one of the two coupling coefficients are zero.
- Using the height of a transmission peak we can infer the ratio of left to right coupling. The width of a transmission peak gives us the sum of the two coupling coefficients.

We can now calculate the current

- Since we have the transmission coefficient

$$T(E)=\frac{\gamma_L\gamma_R}{(E-\epsilon_0)^2+\frac{(\gamma_L+\gamma_R)^2}{4}}$$

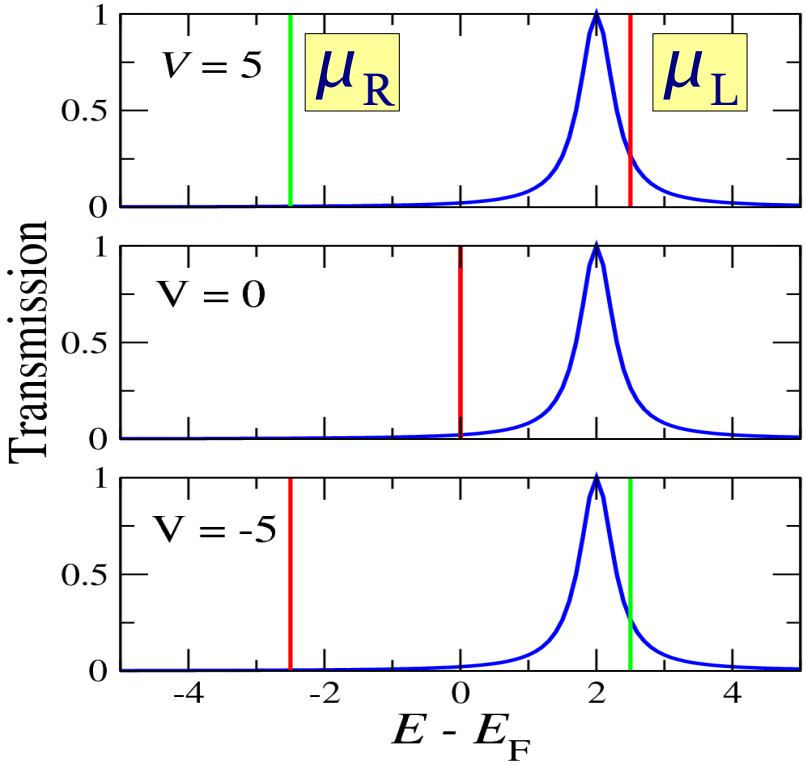
- we can now calculate the current

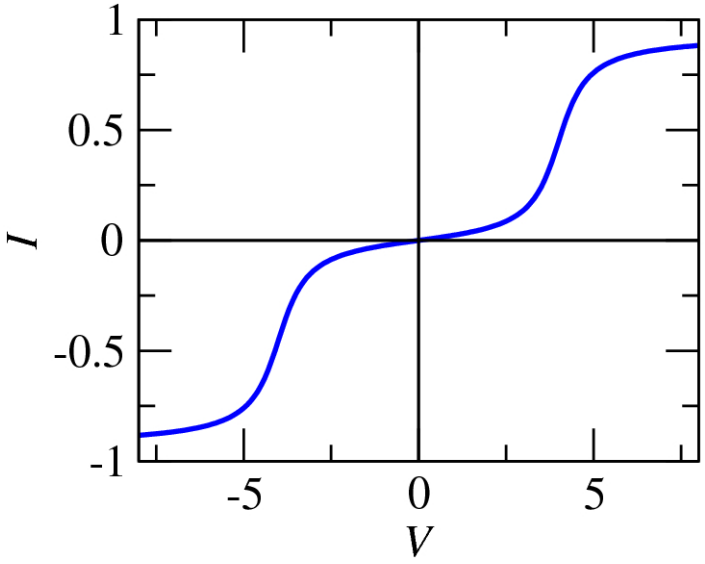
$$I(V)=\frac{e}{h}\int_{\frac{-eV}{2}}^{\frac{eV}{2}} dE\ \ T(E)$$

- For this system we can solve this analytically...

$$I(V)=\frac{2\gamma_L\gamma_R}{\gamma_L+\gamma_R}\left[\arctan\left(\frac{eV-2\epsilon_0}{\gamma_L+\gamma_R}\right)+\arctan\left(\frac{eV+2\epsilon_0}{\gamma_L+\gamma_R}\right)\right]$$

We can now calculate the current





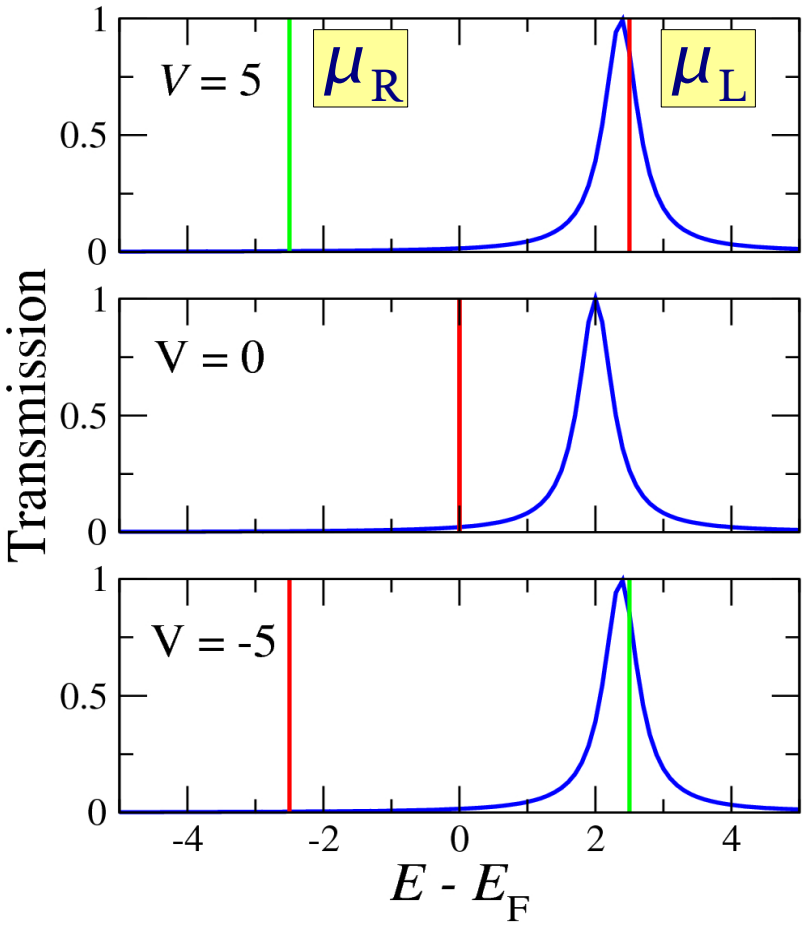
- The current is symmetric for positive and negative bias
- At V = 4 the bias is big enough so that the level enters the bias window and conducts (the conductance gap is therefore $V_{gap} = 8$)
- The current saturates above V = 5

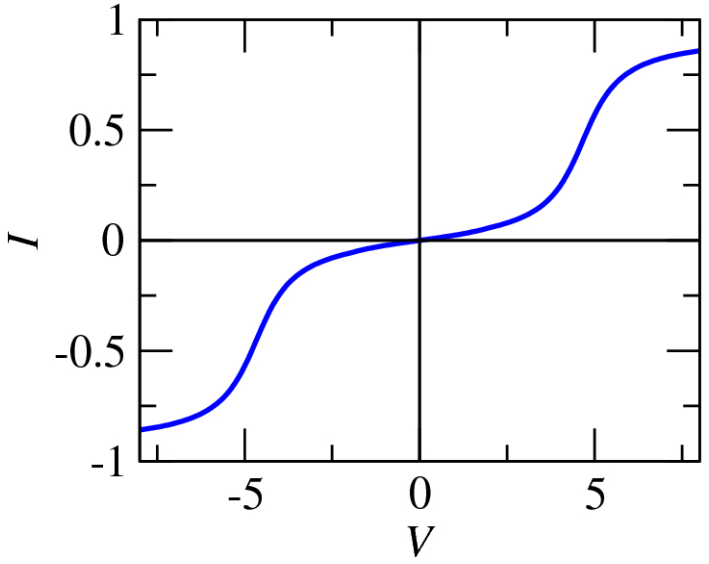
Usually *T(E)* is bias dependent: *T=T(E,V)*

The energy of the molecular level usually changes with bias, so that also the transmission is bias dependent

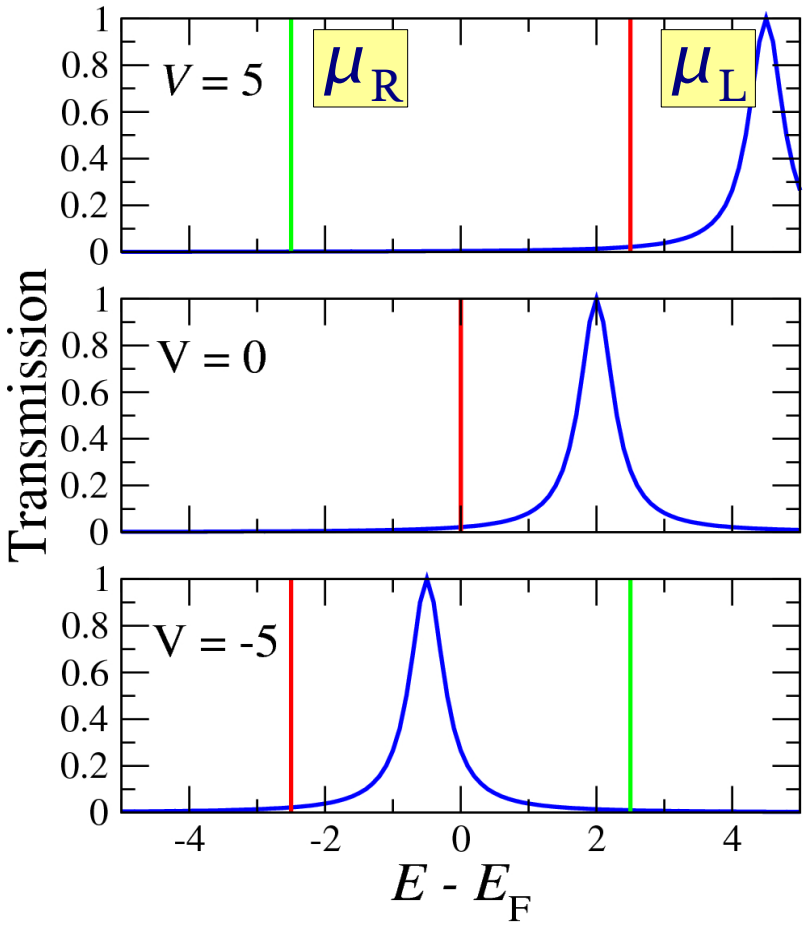
What is the usual bias dependence of T(E,V)?

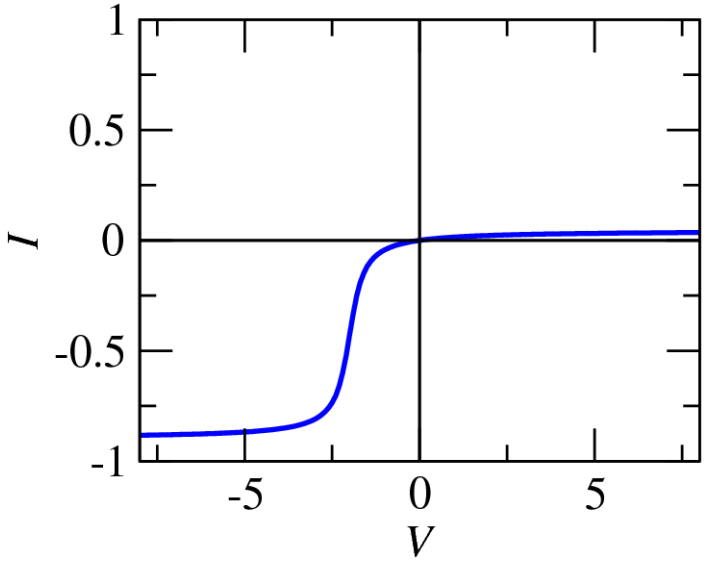
Possiblity 2



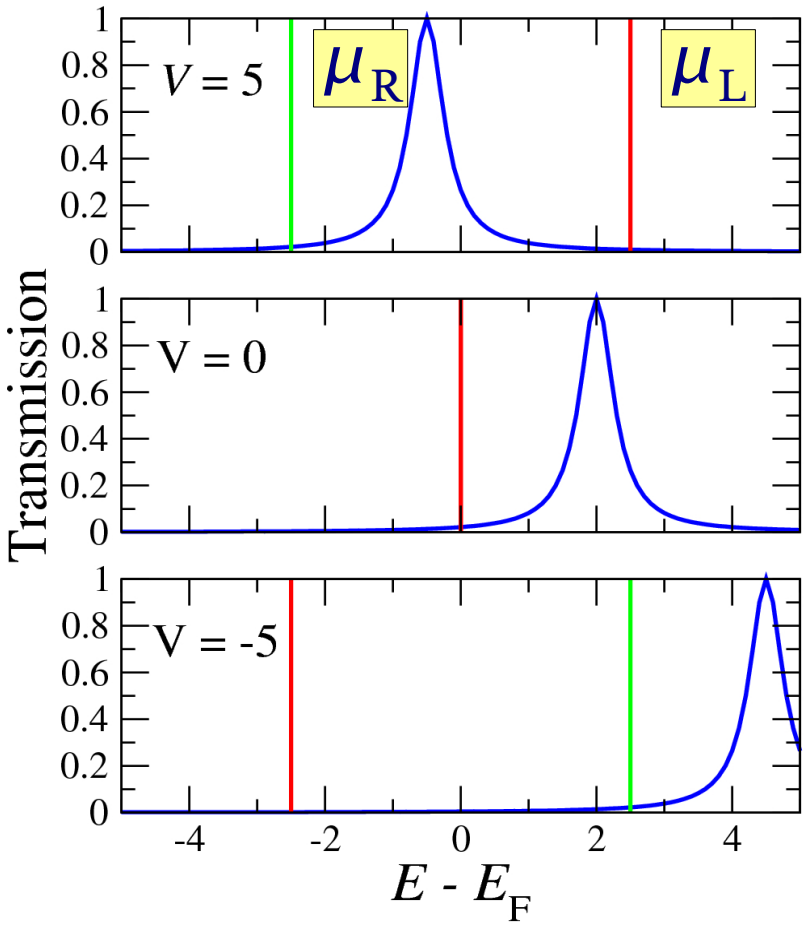


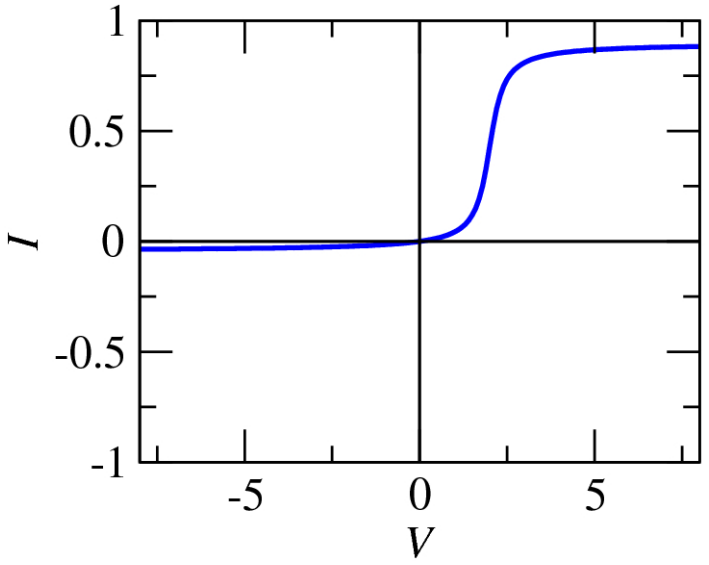
Possiblity 3



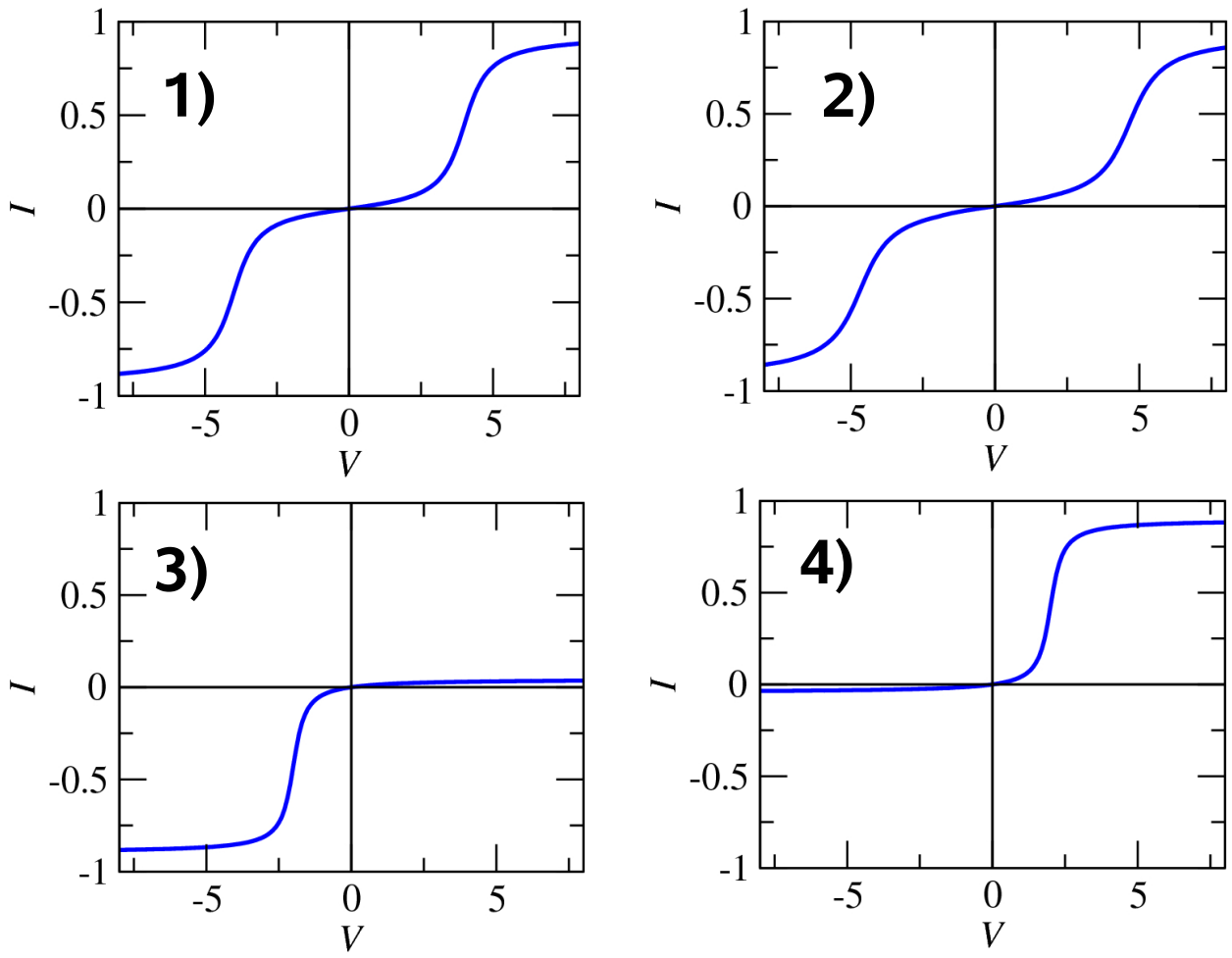


Possiblity 4





Different possible *I-Vs* for the same 0-bias result



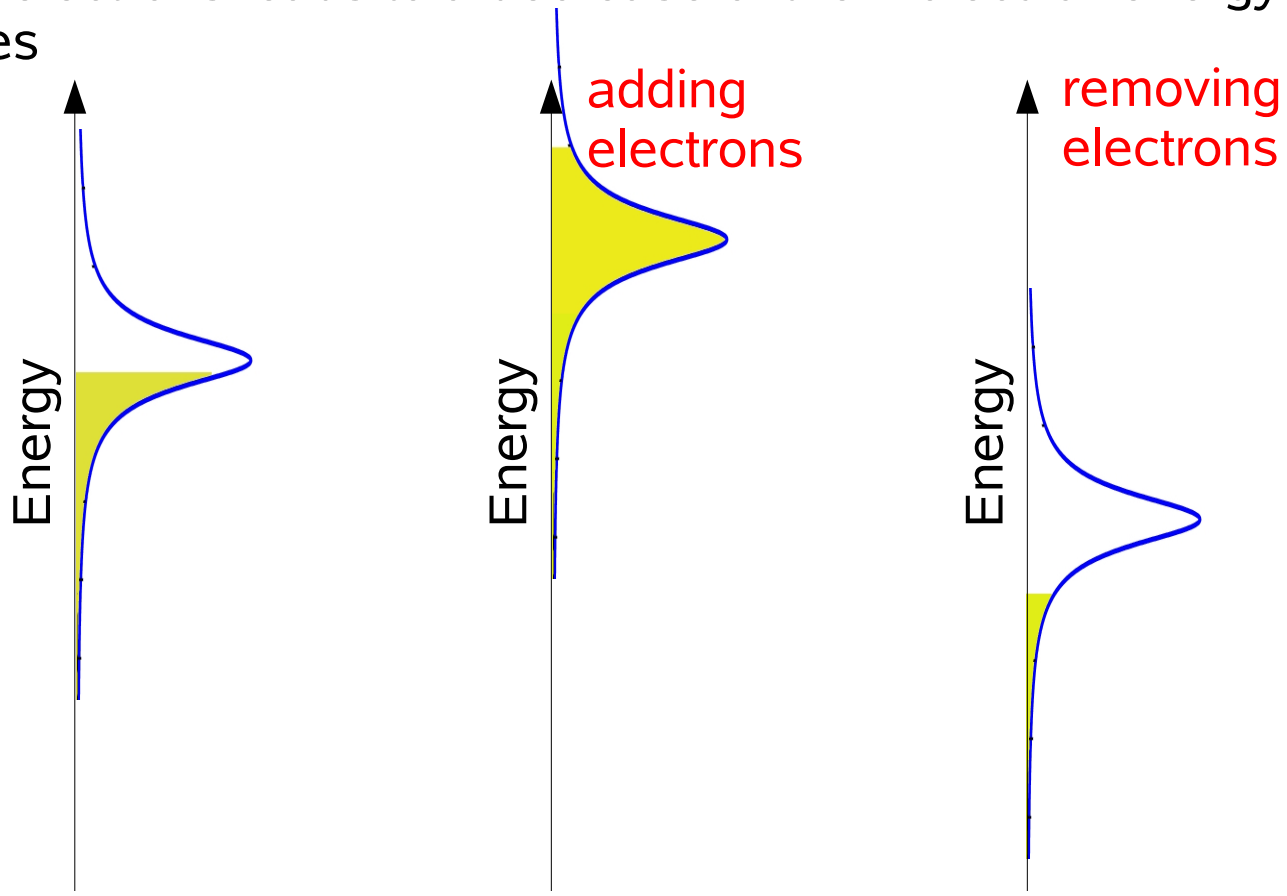
It is crucial to calculate the correct bias dependent position of the molecular levels, in order to obtain the correct *I-V*

What causes the change of the energies of the molecular orbitals with bias?

Charging

The effect of charging on the energy of molecular levels

- Addition of electrons leads to an increase of the molecular energy to higher energies
- Removal of electrons leads to a decrease of the molecular energy to lower energies



How do we calculate the charge? Using NEGF!

Remember...

$$N = \mathrm{Tr}[\rho S]$$

where the density matrix is then obtained as

$$\rho = \frac{1}{2\pi i}\int dE\ G^{<}(E)$$

and with the lesser Green's function defined as

$$G^{<}(E) = i G[f(E-\mu_{\mathrm{L}})\Gamma_{\mathrm{L}} + f(E-\mu_{\mathrm{R}})\Gamma_{\mathrm{R}}]G^{\dagger}$$

f_{L} f_{R}

For our single level system:

The occupation number is equal to the density matrix, since this is just a number for 1 orbital:

$$N = \mathrm{Tr}[\rho S] = \rho$$

Using the previous result for the Green's function

$$G(E) = \frac{1}{E - \epsilon_0 + i\frac{\gamma_L + \gamma_R}{2}}$$

the lesser Green's function becomes

$$G^<(E) = i G[f_L \Gamma_L + f_R \Gamma_R] G^\dagger$$

$$= i \frac{1}{E - \epsilon_0 + i\frac{\gamma_L + \gamma_R}{2}} [f_L \gamma_L + f_R \gamma_R] \frac{1}{E - \epsilon_0 - i\frac{\gamma_L + \gamma_R}{2}}$$

For our single level system:

The lesser Green's function can be written as

$$G^{<}(E) = i \frac{1}{E - \epsilon_0 + i\frac{\gamma_L + \gamma_R}{2}} \left[f_L \gamma_L + f_R \gamma_R \right] \frac{1}{E - \epsilon_0 - i\frac{\gamma_L + \gamma_R}{2}}$$

$$= i \underbrace{\frac{\gamma_L + \gamma_R}{(E - \epsilon_0)^2 + \frac{(\gamma_L + \gamma_R)^2}{4}}}_{\mathrm{DOS}(E)} \underbrace{\frac{f_L \gamma_L + f_R \gamma_R}{\gamma_L + \gamma_R}}_{p(E)}$$

$$= 2\pi i \qquad \mathrm{DOS}(E) \qquad p(E)$$

$p(E)$ → **Occupation probability**

Occupation probability

$$p(E)=\frac{f_L\gamma_L+f_R\gamma_R}{\gamma_L+\gamma_R}$$

We now analyze 4 possible cases for *p(E)*:

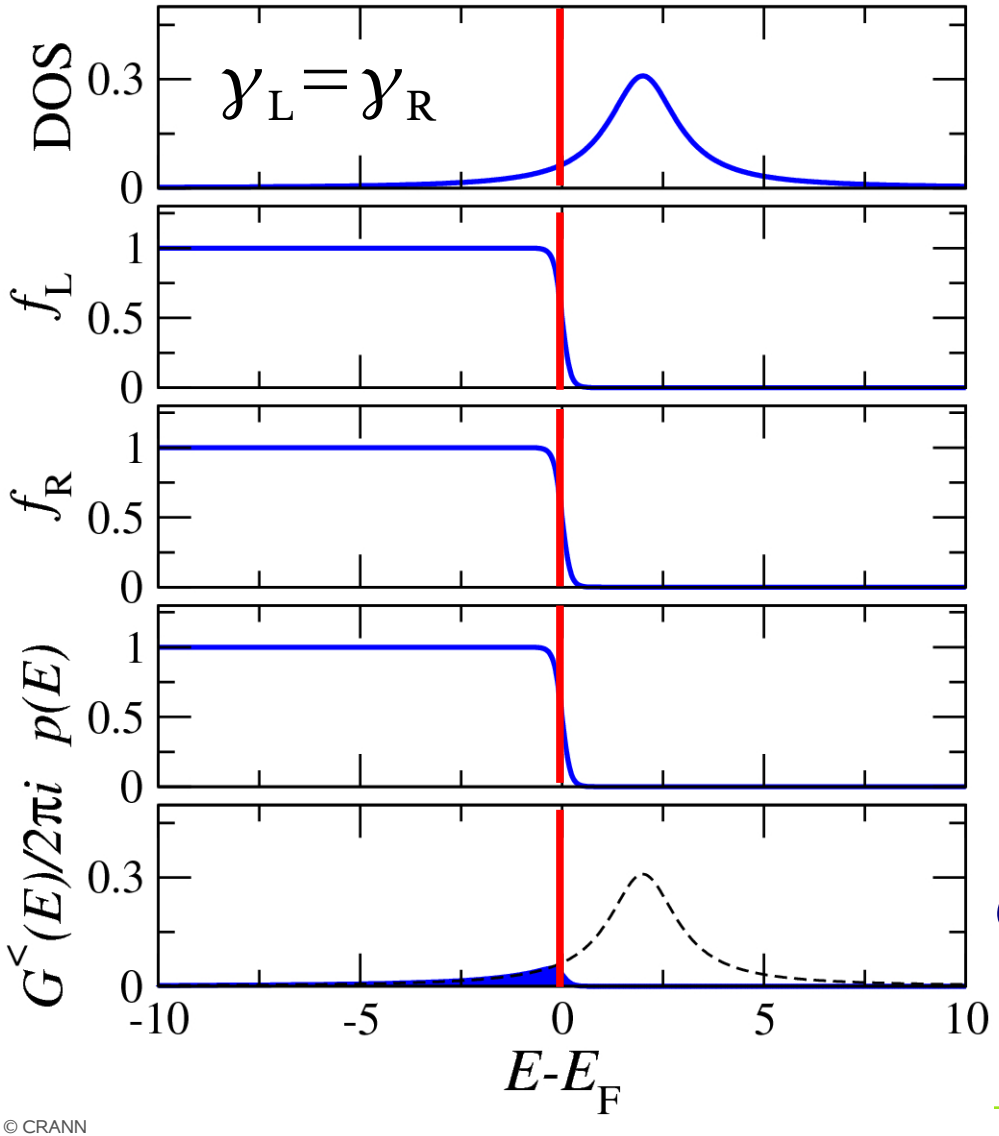
1) $f_L=f_R\approx 1 \longrightarrow p\approx 1$

2) $f_L=f_R\approx 0 \longrightarrow p\approx 0$

3) $f_L\approx 1\ ,\ f_R\approx 0 \longrightarrow p=\frac{\gamma_L}{\gamma_L+\gamma_R}$

4) $f_L\approx 0\ ,\ f_R\approx 1 \longrightarrow p=\frac{\gamma_R}{\gamma_L+\gamma_R}$

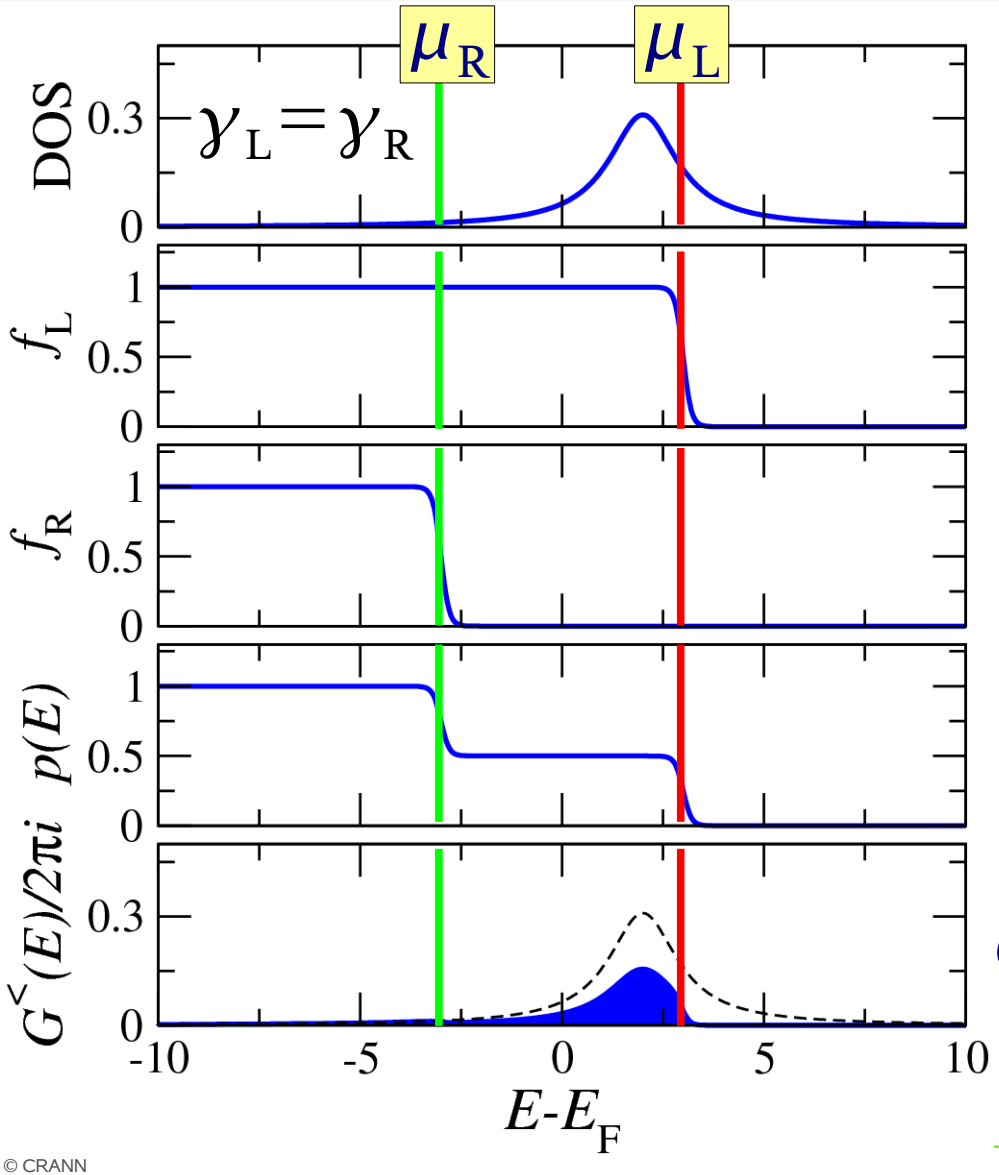
Occupation probability: V_b=0



$$p(E) = \frac{f_L \gamma_L + f_R \gamma_R}{\gamma_L + \gamma_R}$$

$$G^<(E) = 2\pi i \, \mathrm{DOS}(E) \, p(E)$$

Occupation probability: V_b=6

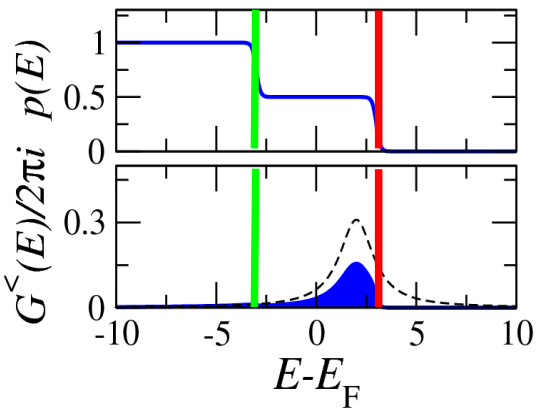


$$p(E) = \frac{f_L \gamma_L + f_R \gamma_R}{\gamma_L + \gamma_R}$$

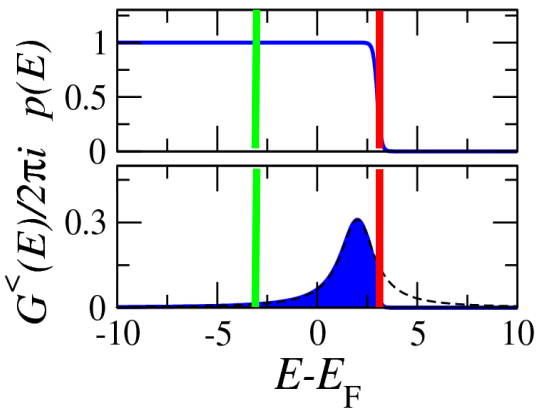
$$G^<(E) = 2\pi i \, \mathrm{DOS}(E) \, p(E)$$

Effect of asymmetric coupling (V_b=6)

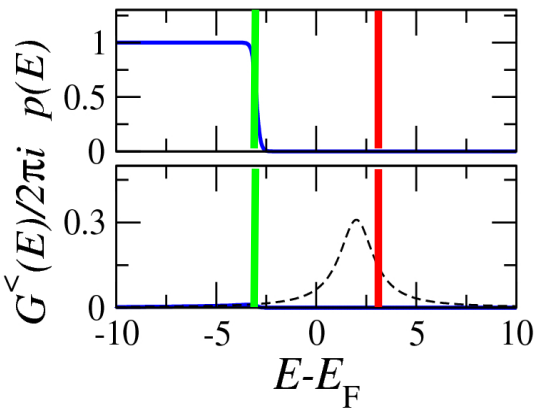
$\gamma_L = \gamma_R$



$\gamma_L \gg \gamma_R$



$\gamma_L \ll \gamma_R$



$$p(E) = \frac{f_L \gamma_L + f_R \gamma_R}{\gamma_L + \gamma_R}$$

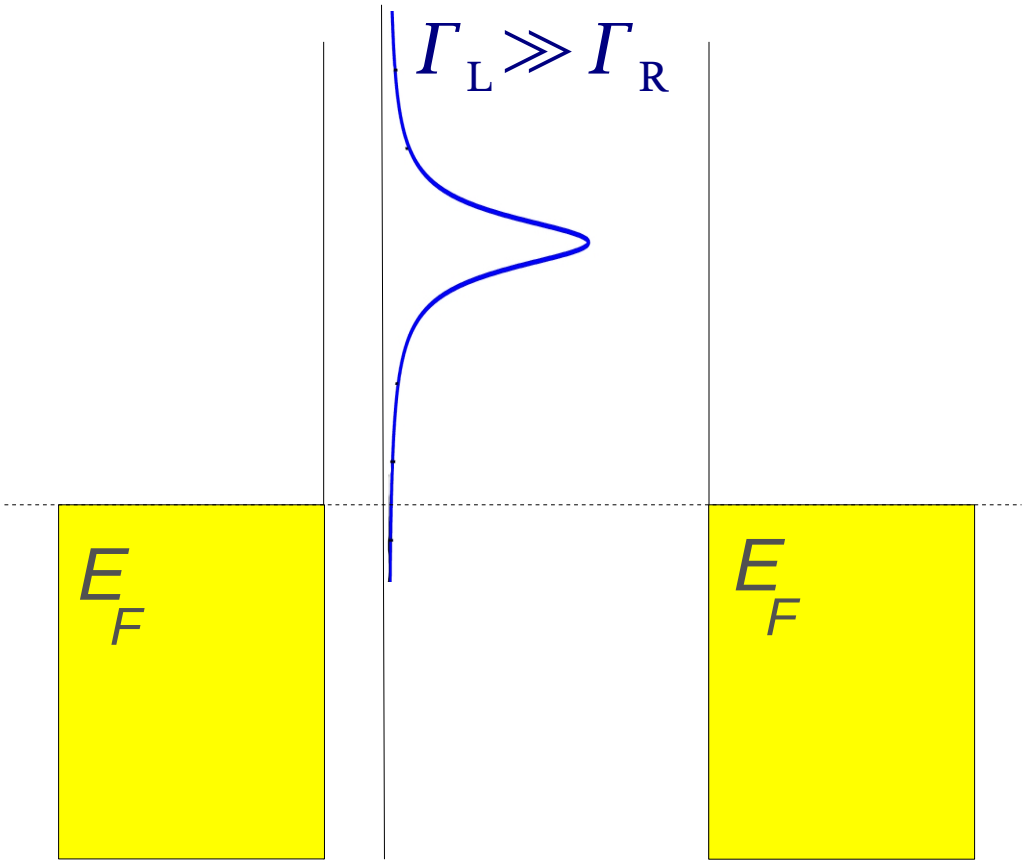
$$G^<(E) = 2\pi i \, \mathrm{DOS}(E)\, p(E)$$

- The charging depends on the ratio of the two coupling coefficients γ_L and γ_R

Self-consistent calculation of the energy level

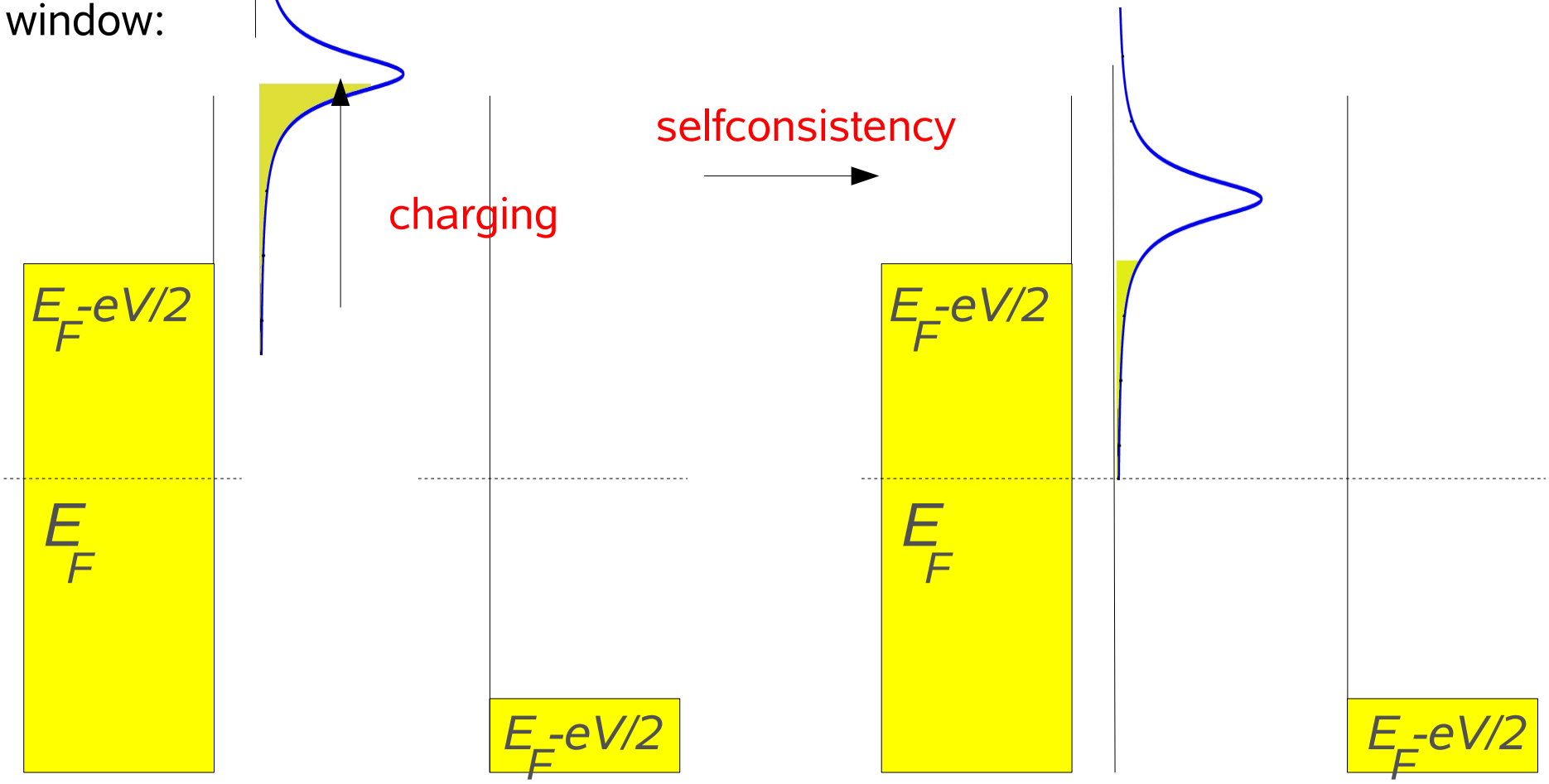
We start with an empty level, broadened by the contact to the leads

We assume that the coupling to the left is much larger than the coupling to the right side

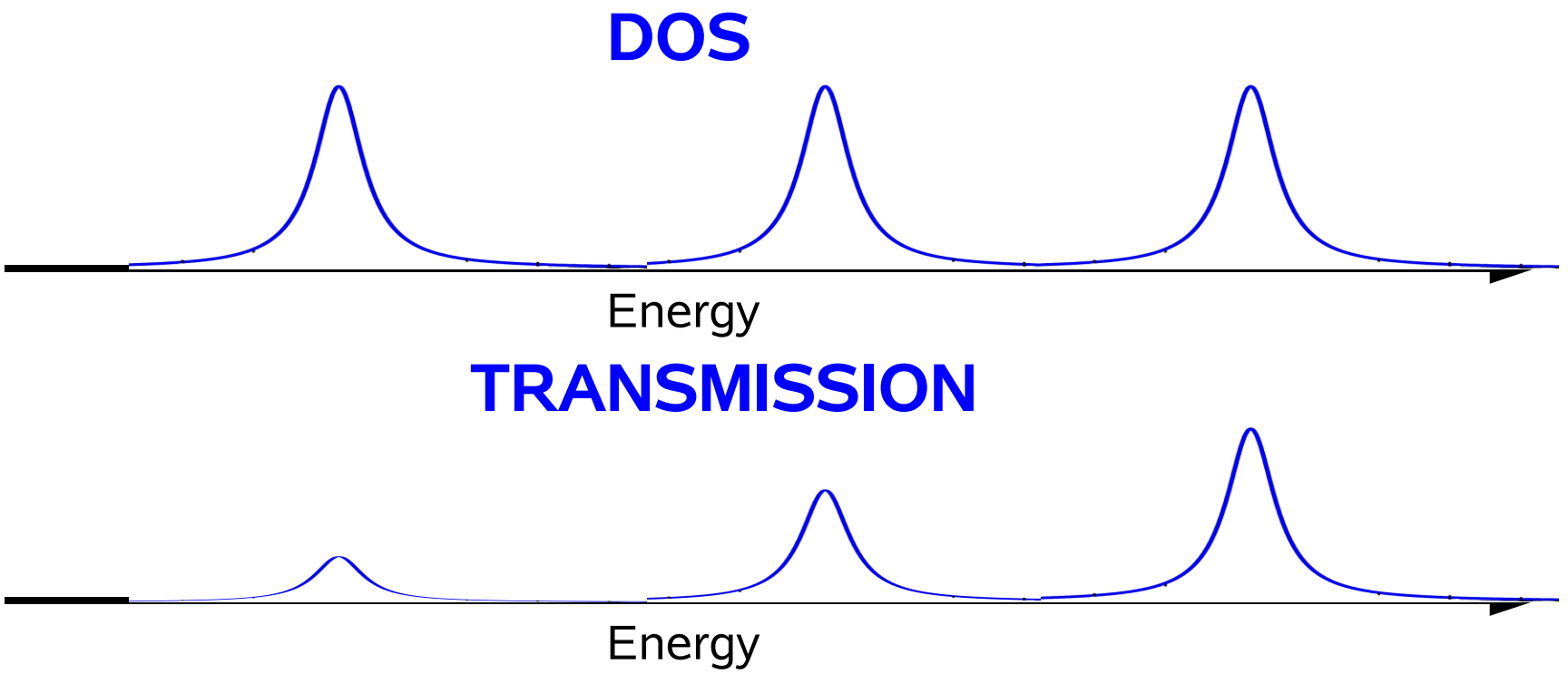


The effect of charging on the energy of molecular levels

We now apply a bias large enough, so that part of the level is in the bias window:

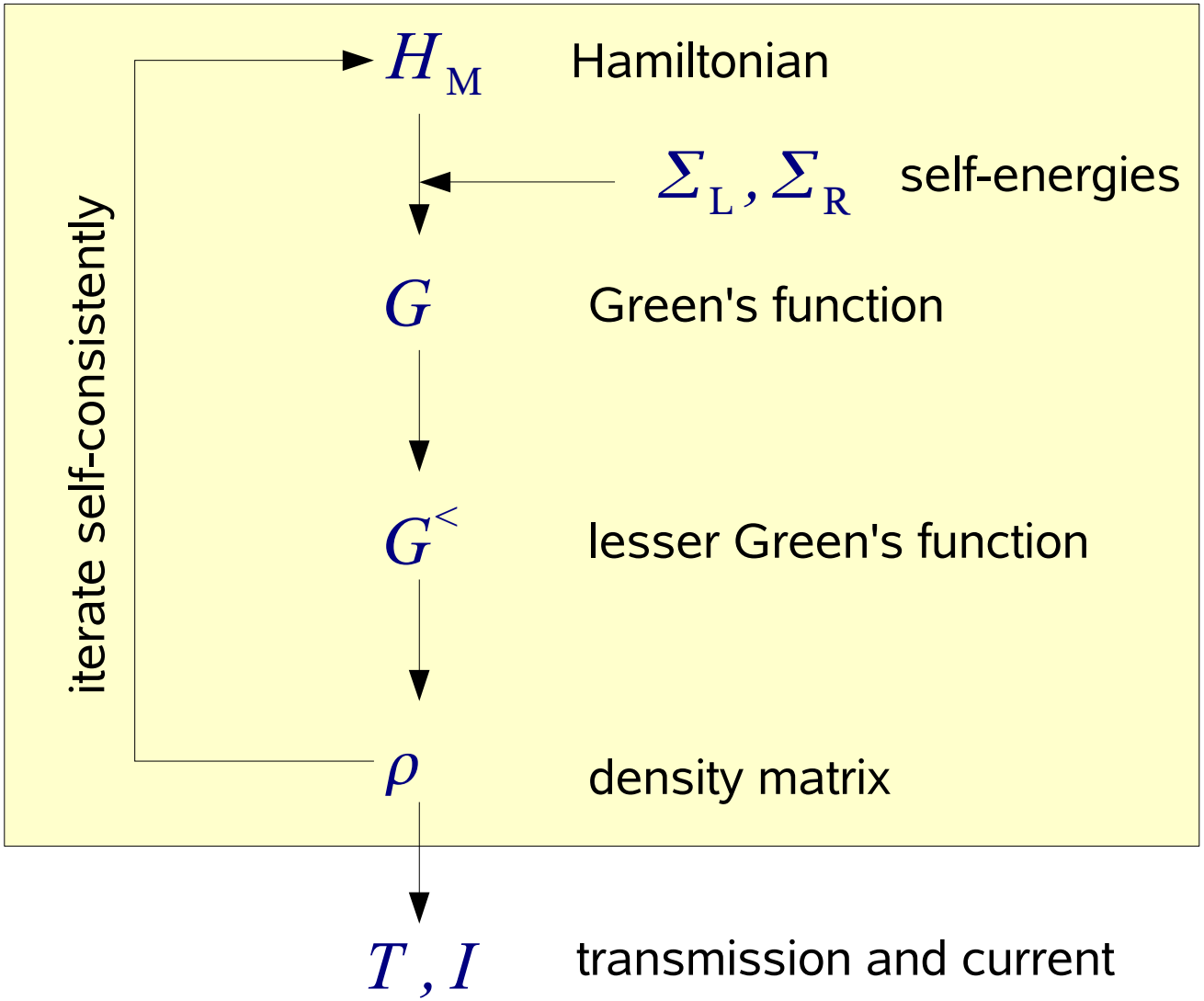


From a single level to multiple levels

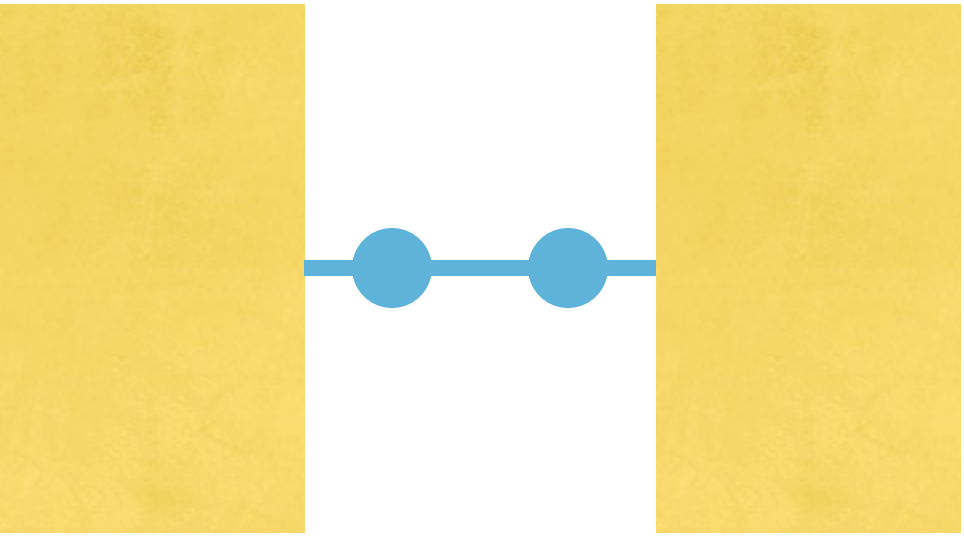


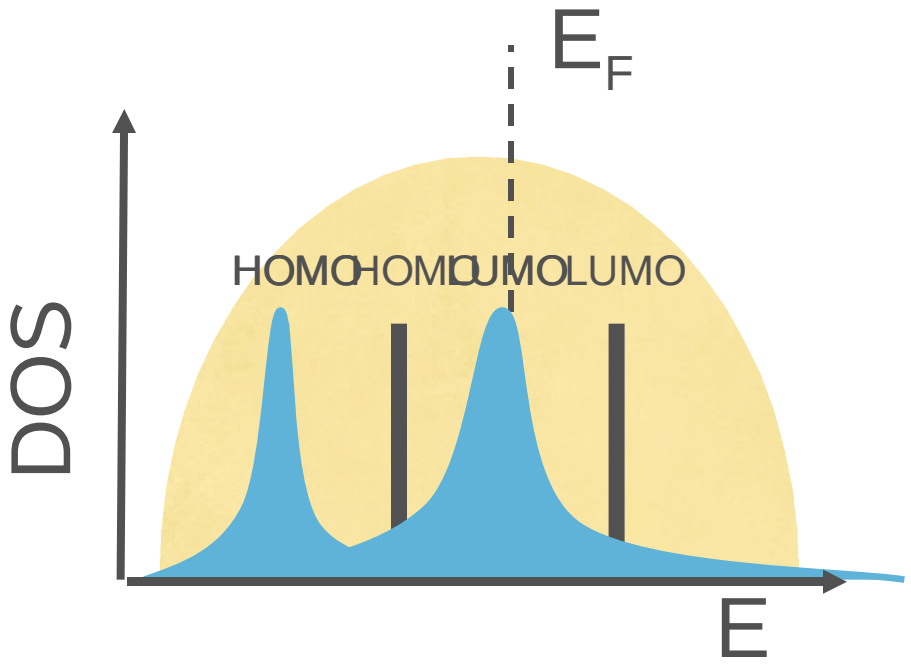
- If the levels are well separated, then the solution is simply the superpositions of single level results
- If the levels are close together, so that they overlap, then there will be additional interference effects

NEGF + DFT



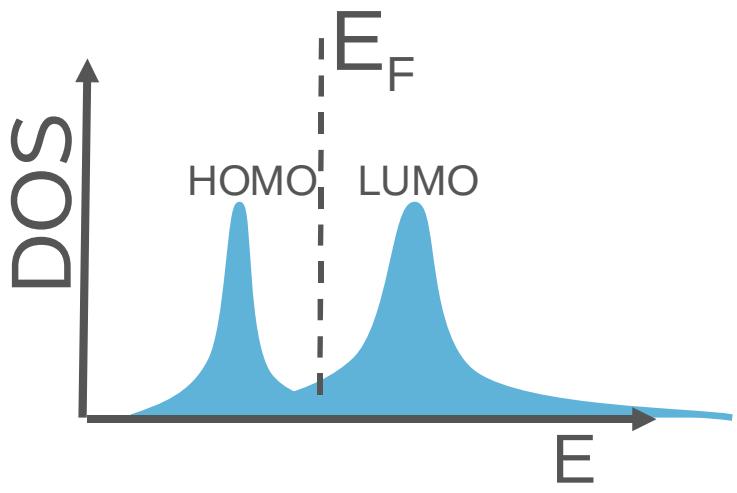
Schematic level alignment



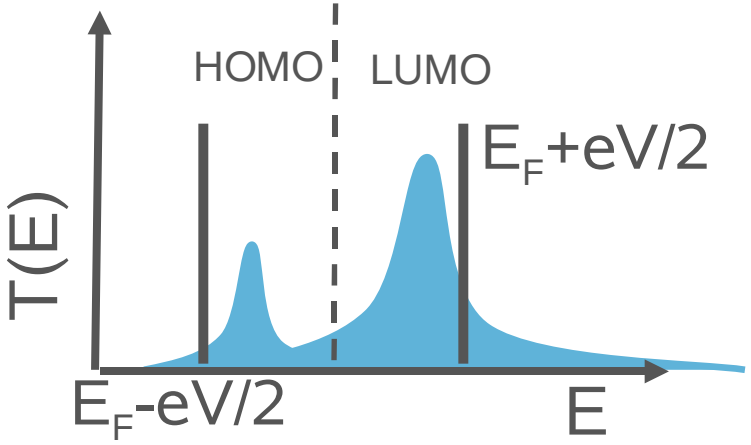


$$H_M + \mathrm{Re}\Sigma + \mathrm{Im}\Sigma$$

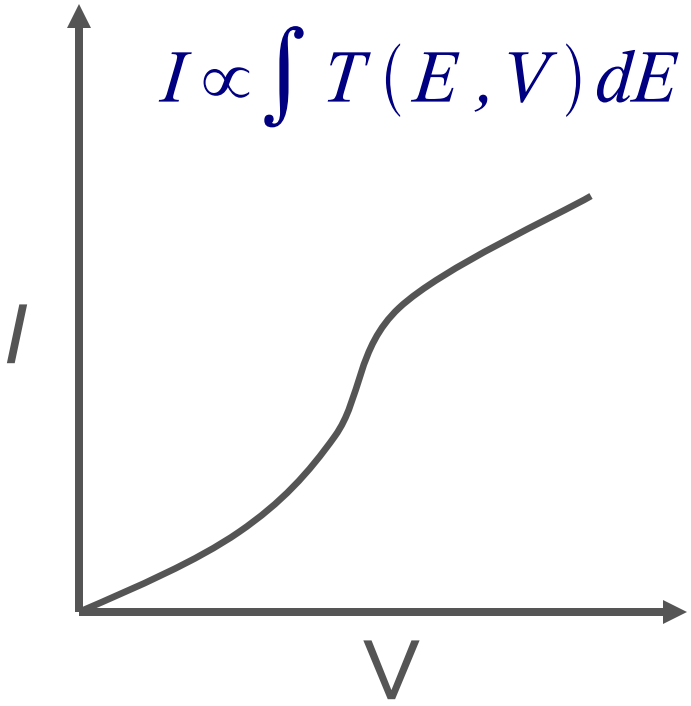
Schematic I-V



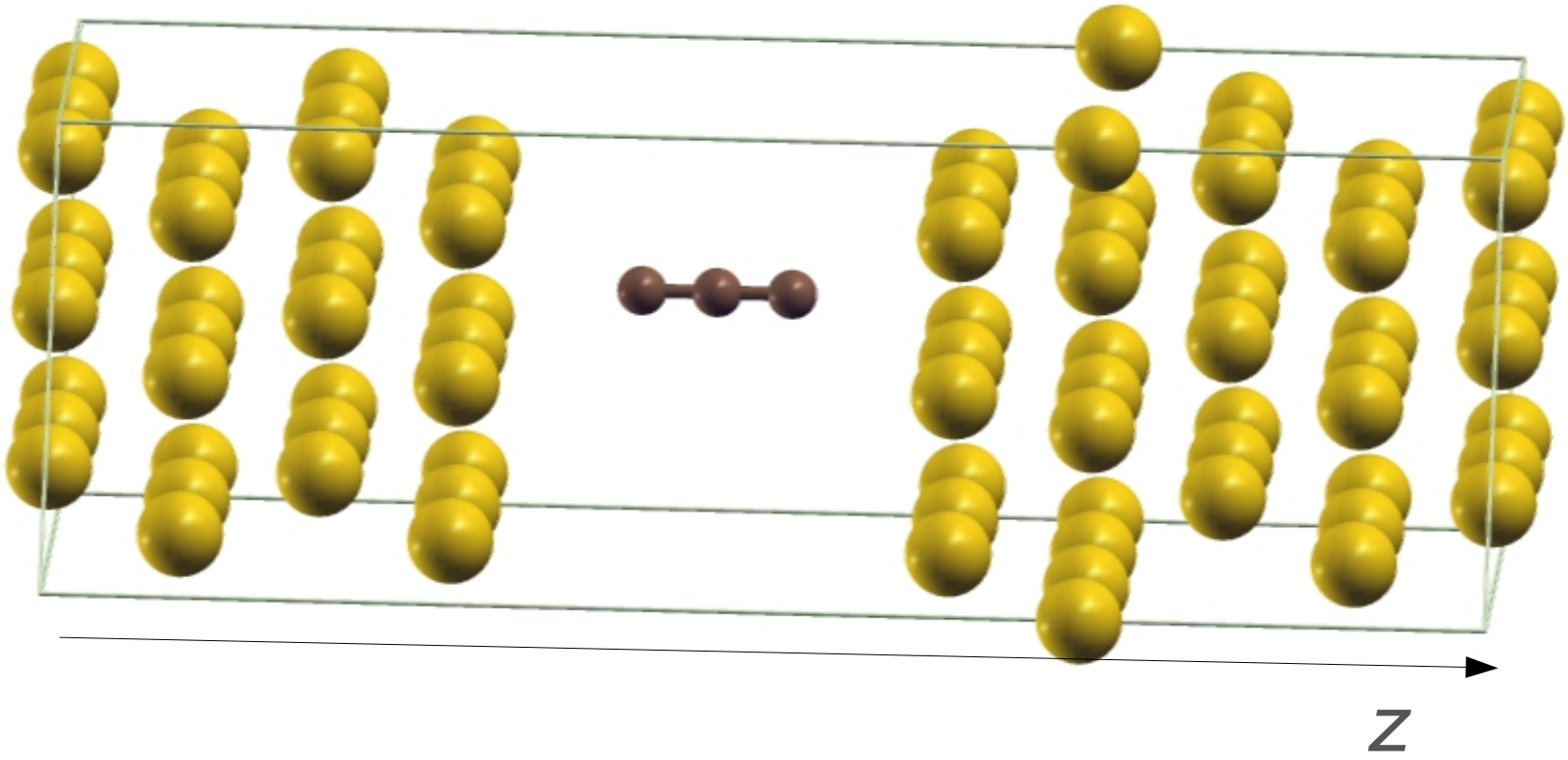
$$T \propto \mathrm{DOS} \times \mathrm{Im}(\Sigma)^2$$



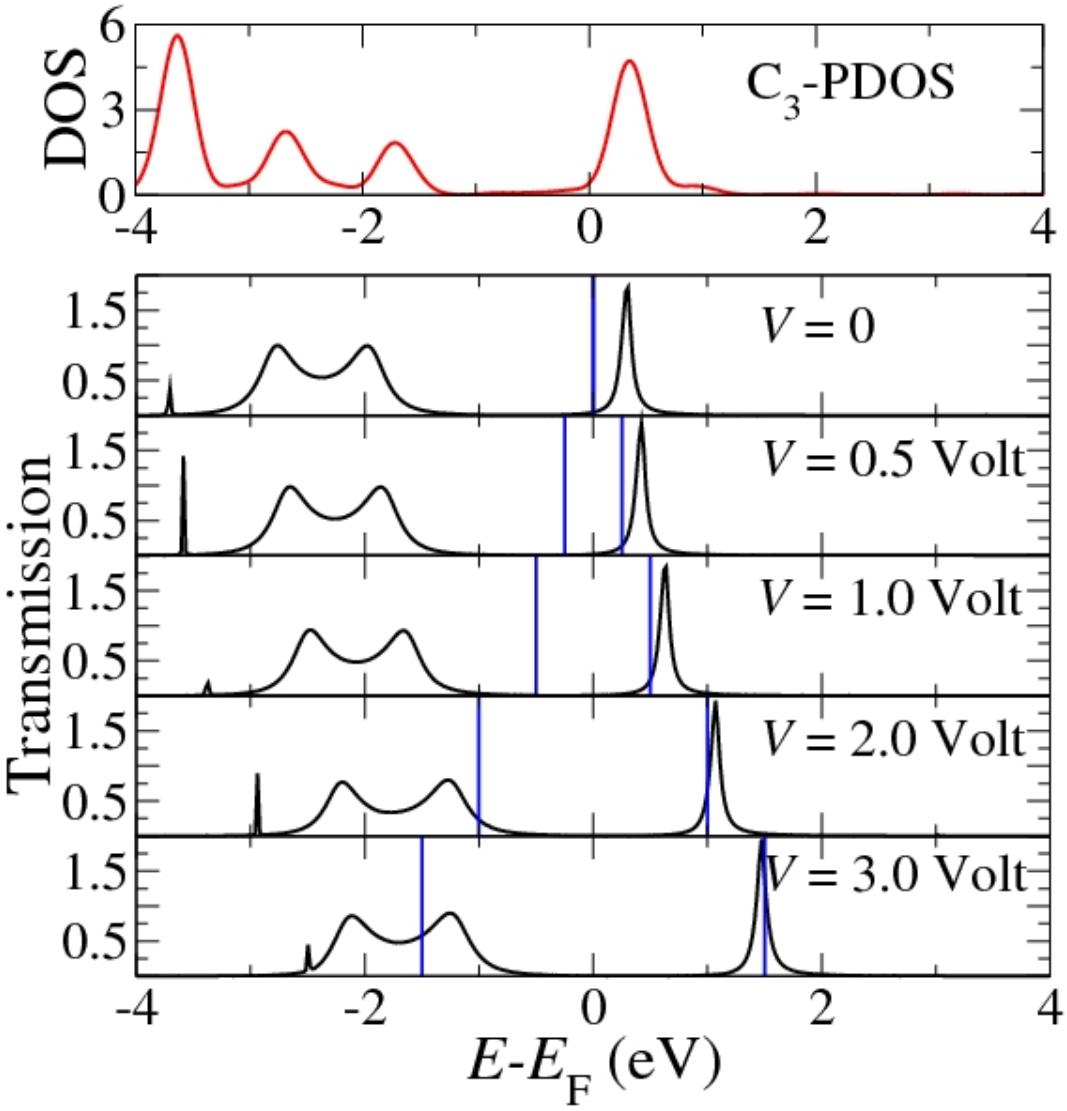
$$I \propto \int T(E,V)\,dE$$

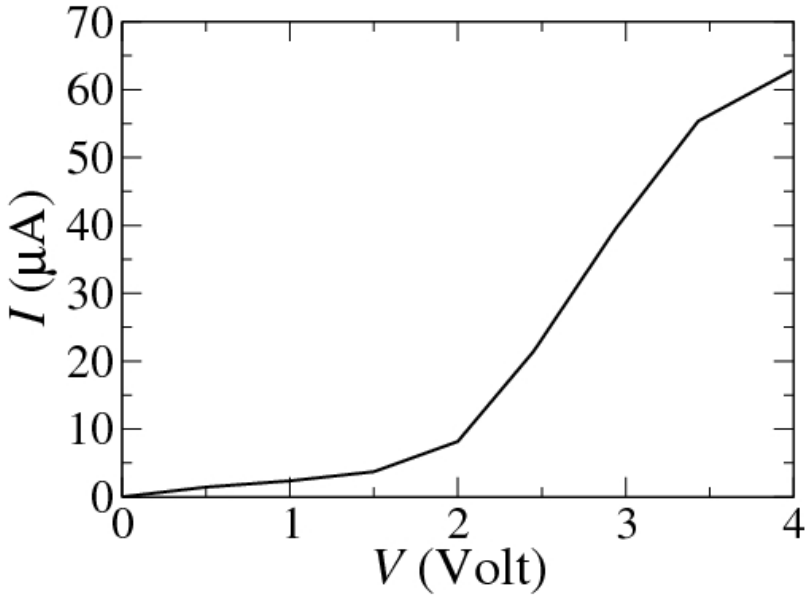


This will be done at the practical tutorial

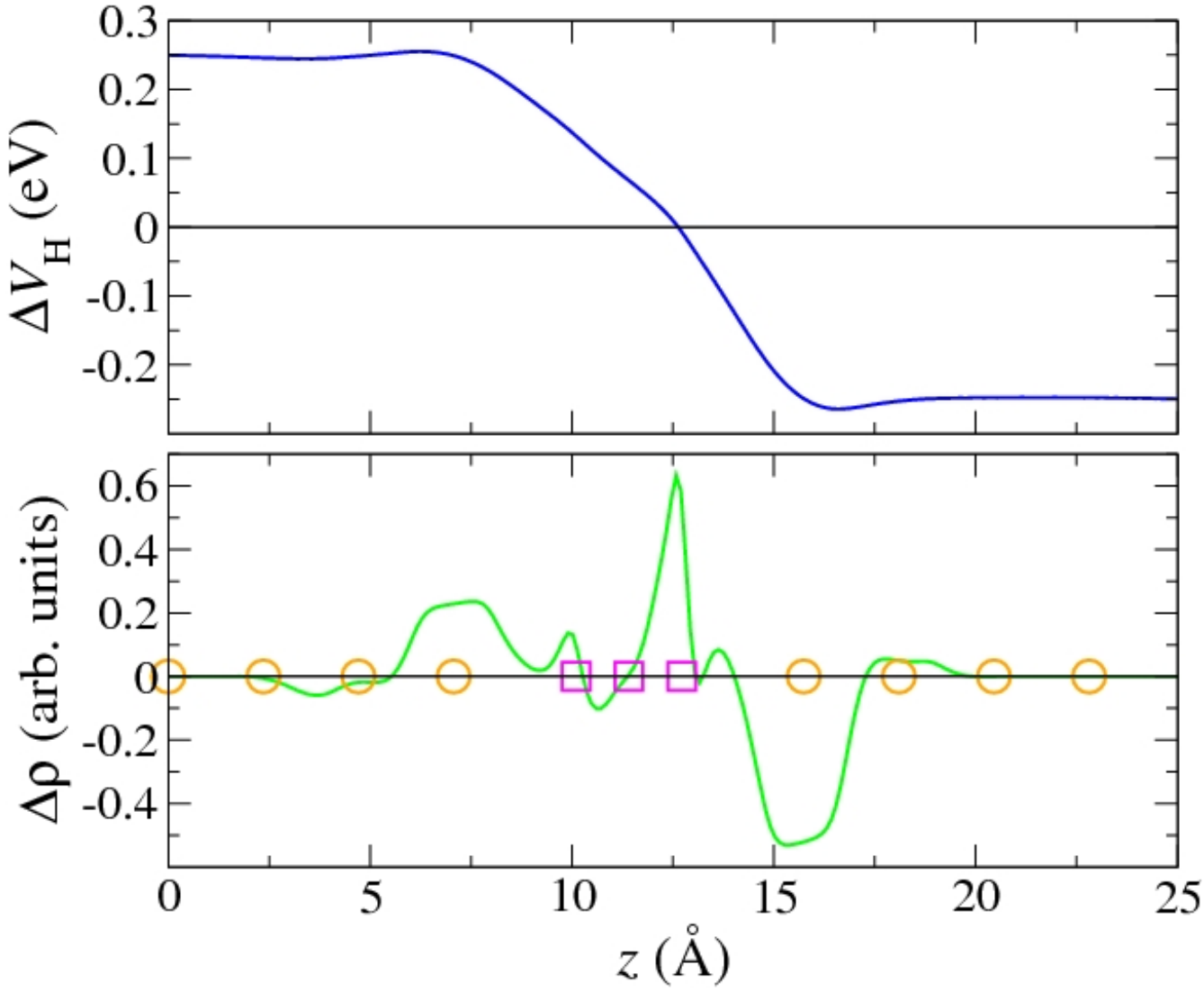


Bias dependent transmission and I-V





Potential drop and charging



Tutorial

- As next step you will calculate a few real systems, and analyze the data, with special attention to the quantities presented in the lecture