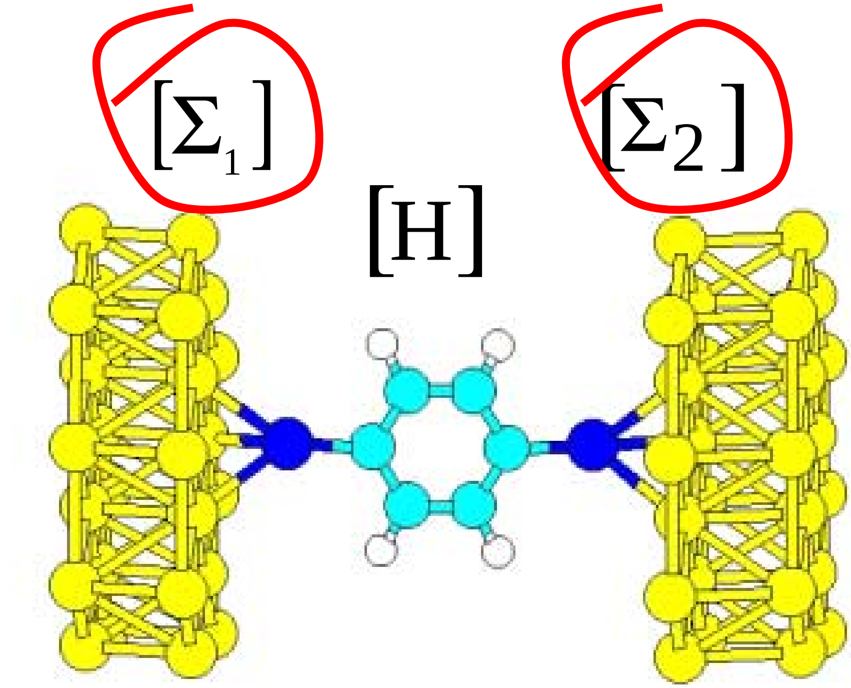
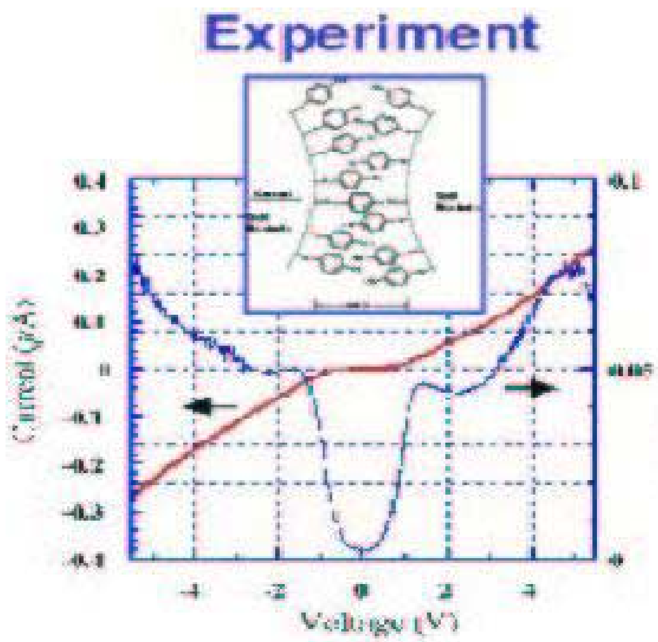
Modeling Contacts

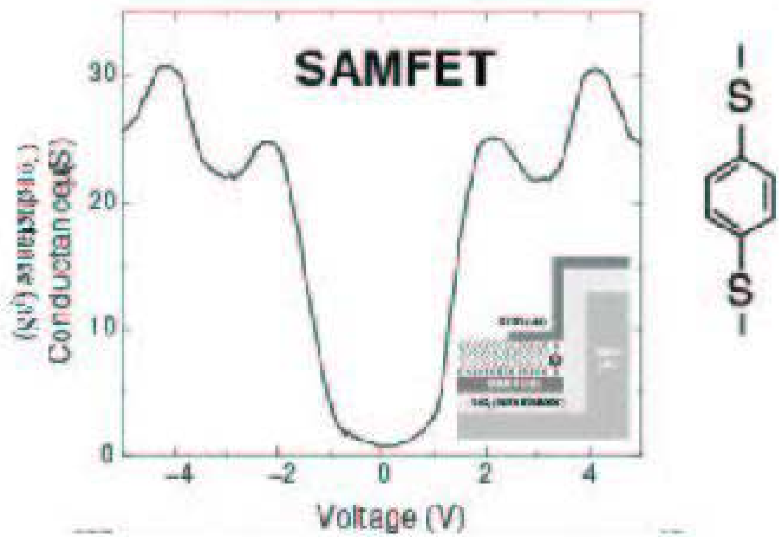


Titash Rakshit

Same Molecule: Different I-V

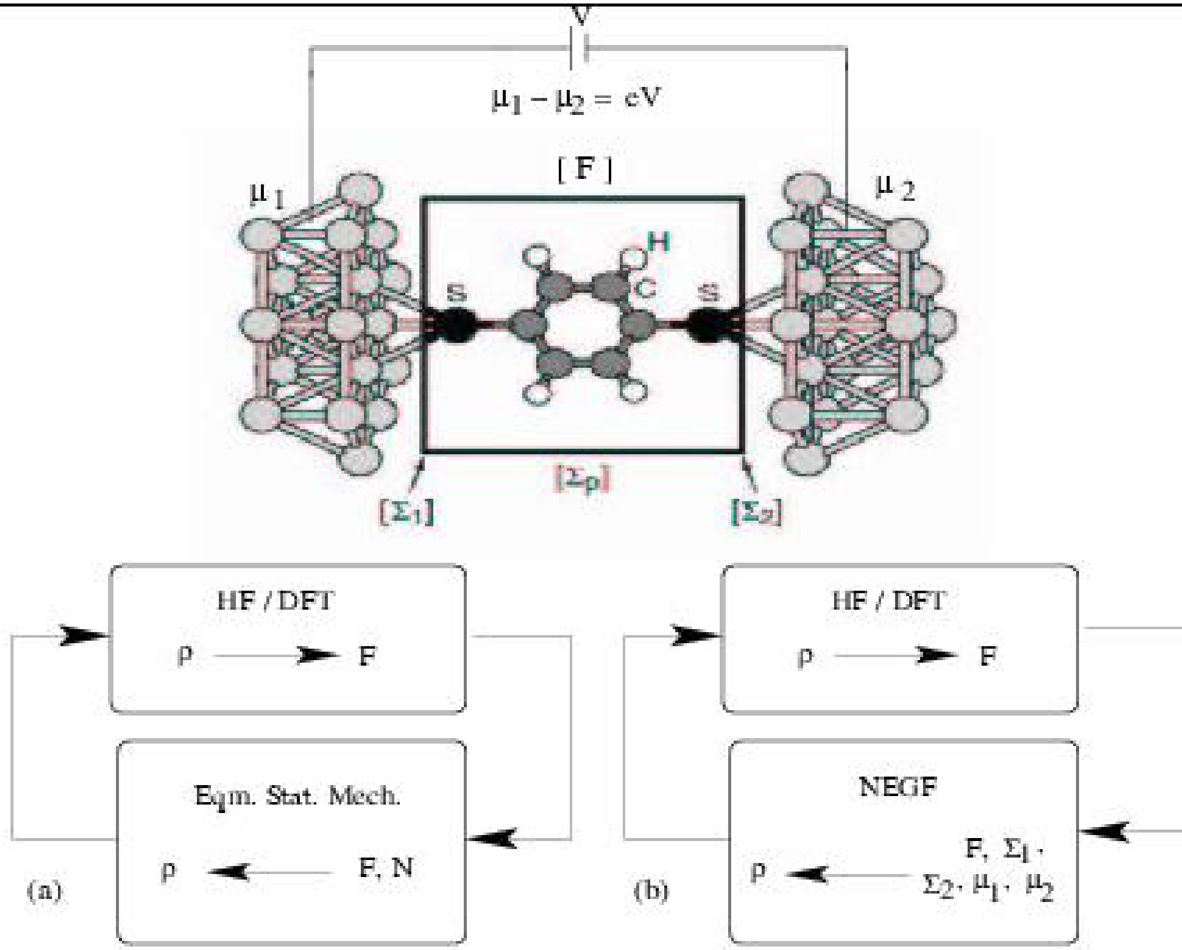


[Reed *et al.*, '97]



[Schön *et al.*, '02]

Contact: Adds self-energy to H



Green's Function

Green's Function gives an **impulse response** to the Schrodinger equation at any point due to an excitation at any other point

$$\text{instead of} \quad H\psi = E\psi$$

$$\text{we can write} \quad (E-H)G(E) = I$$

$$I = \text{identity matrix}$$

$$G(E) \Rightarrow \begin{array}{ll} \text{retarded} & \text{causal} \\ \text{advanced} & \text{non-causal} \end{array}$$

Partitioning Scheme

$$\begin{bmatrix} H_d & \tau \\ \tau^+ & H_c \end{bmatrix}$$: **size** of matrix huge

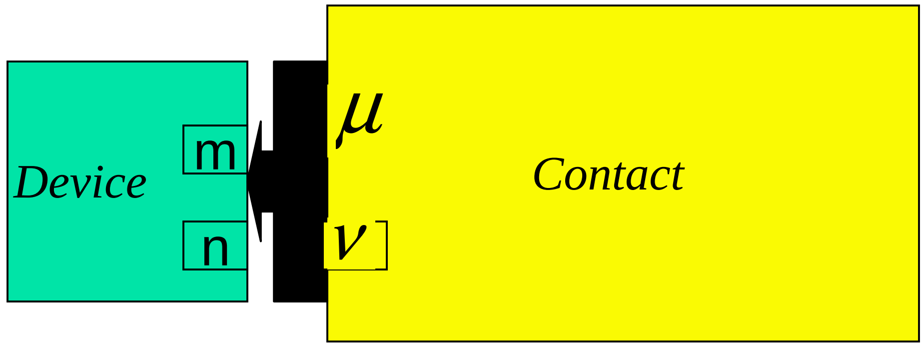
$$\begin{bmatrix} G_d & G_{dc} \\ G_{cd} & G_c \end{bmatrix} = \begin{bmatrix} (E+i0^+)I - H_d & -\tau \\ -\tau^+ & (E+i0^+)I - H_C \end{bmatrix}^{-1}$$

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

$$\Sigma = \tau G_c \tau^+$$: **Self Energy**

Interested in **G** of device only

Do we need to find infinite G_c ?



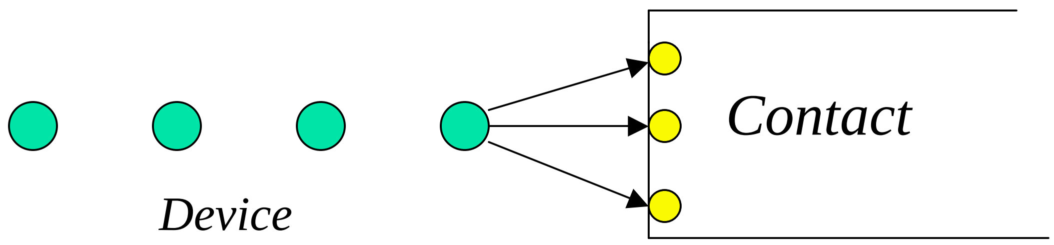
$$\Sigma(m,n) = \sum_{\mu,\nu} \tau(m,\mu) G_c \tau^+(\nu,n)$$

Non-zero element of $\Sigma(m,n)$ only when (m,n) has **overlap** with (μ,ν)

Essentially solving : $\Sigma = \tau g_c \tau^+$ g_c :**surface green's function**

Surface Green's Function much smaller than G_c

What is the size of sigma?



$$\textbf{size of } \tau \Rightarrow 1\times 3 \qquad \textbf{size of } g_c \Rightarrow 3\times 3$$

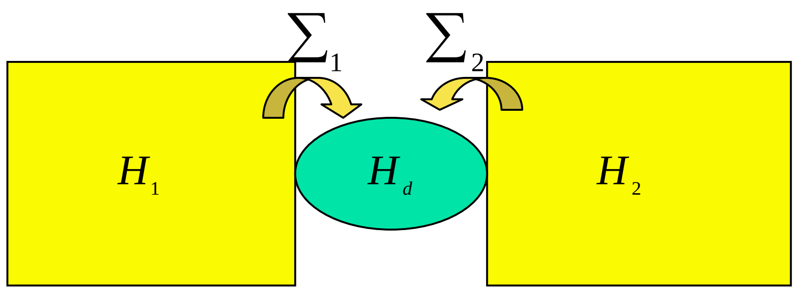
$$\textbf{size of } \Sigma = \tau g_c \tau^+ \Rightarrow 1\times 1 \qquad \textbf{size of } d\textbf{evice Hamiltonian } (\mathbf{H_d}) \Rightarrow 4\times 4$$

$$\overline{\Sigma} = \begin{bmatrix} \tau g_c \tau^+ & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\mathbf{H_{eff}} = \mathbf{H_d} + \overline{\Sigma}$$

Self-Energy: Advantages

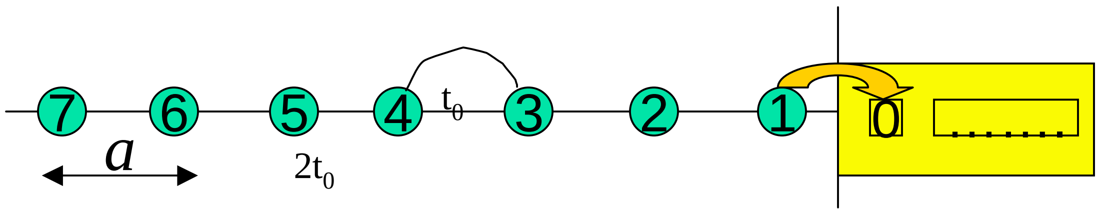
Effect of Semi-infinite contacts: as **small** as the size of the **Device** Hamiltonian !!!



Effective Device Hamiltonian : $H_{eff} = H_d + \Sigma_1 + \Sigma_2$

$\Sigma_1 \quad \Sigma_2$ **: Same size as** H_d

Getting the Surface Green's Function



1-D lattice, 1-D contacts

$$\Sigma(1,1) = \tau(1,0)g_c\tau^+(0,1) = t_0^{\,2}g_c(0,0)$$

$$\begin{bmatrix} g_c(0,0) & .... \\ g_c(-1,0) & .... \\ .... & ...... \end{bmatrix}\begin{bmatrix} E+i0^+-2t_0 & t_0 & .... & \\ t_0 & E+i0^+-2t_0 & t_0 & .... \\ .... & .... & .... & \end{bmatrix} = \begin{bmatrix} 1 & 0 & ...... \\ 0 & 1 & ...... \\ ... & ... & .... \end{bmatrix}$$

For outgoing waves: $g_c(-1,0) = g_c(0,0)\exp(ika)$

Surface green's function: $g_c(0,0) = -\exp(ika)/t_0$

Sigma is a Complex Quantity

For a 1-D lead: $\Sigma(1,1) = -t_0 \exp(ika)$

$$\sum = \mathbf{Re}(\sum) + \mathbf{i} \times \mathbf{Im}(\sum)$$

$\mathbf{Re}(\sum) \Rightarrow$ Shifts energy levels up or down

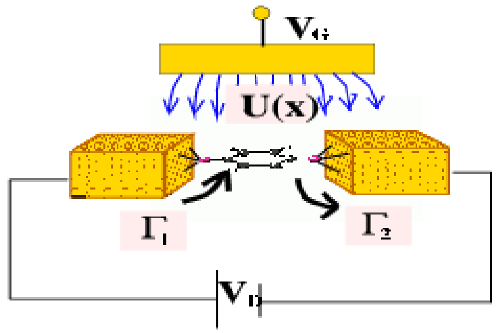
$\mathbf{Im}(\sum) = -t_0 \sin ka = \dfrac{\hbar \nu}{a} \Rightarrow$ Gives a finite lifetime to a carrier in an eigenstate

Electron in an eigenstate does not stay there forever decays through interactions with the contacts:

Fermi's Golden Rule

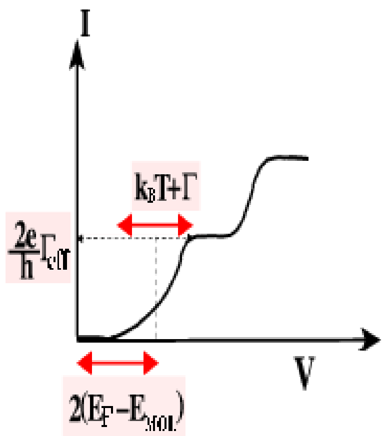
Gamma from Sigma

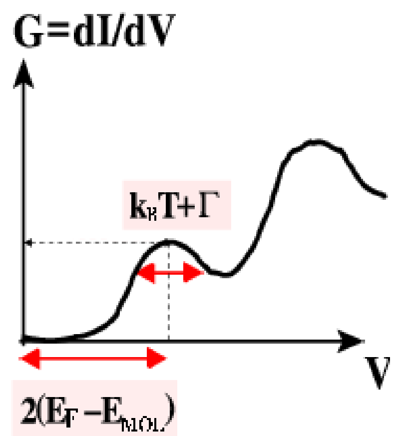
$$\textbf{Broadening}: \; \Gamma = i(\Sigma - \Sigma^{+}) = 2 \times \mathbf{Im}(\Sigma)$$



$\Gamma = \Gamma_1 + \Gamma_2$

$\Gamma_{eff} = \Gamma_1 \Gamma_2 / (\Gamma_1 + \Gamma_2)$

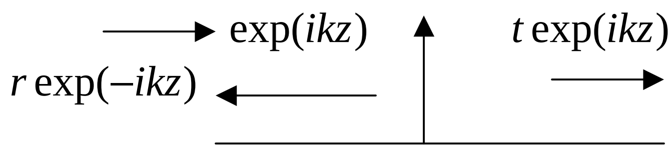




Solving the Schrodinger Equation

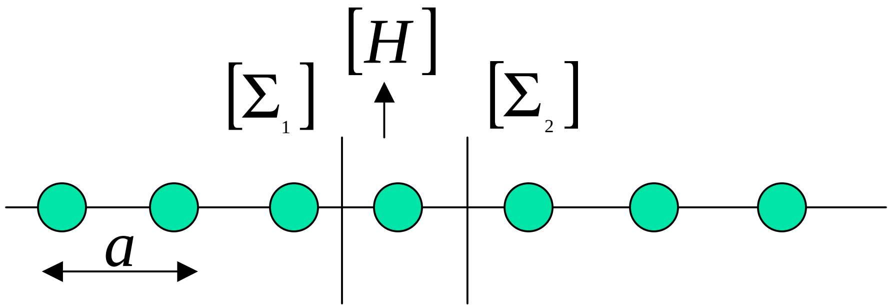
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dz^2}+U_0\delta(z)\psi=E\psi$$

$$[\psi]_{z=0+}=[\psi]_{z=0-}=0\rightarrow t-(1+r)=0 \qquad \left.\frac{d\psi}{dz}\right|_{z=0+}=\left.\frac{d\psi}{dz}\right|_{z=0-}=\left.\frac{2mU_0}{\hbar^2}\psi\right|_{z=0}$$



$$ik[t-(1-r)]=\frac{2mU_0t}{\hbar^2}\rightarrow T(E)=|t|^2=\frac{\hbar\nu(E)^2}{\hbar\nu(E)^2+U_0{}^2}$$

Same Problem: Using Green's Function



$$[H] = 2t_0 + U_0 / a$$

$$\Sigma_1(E) = -t_0 e^{(ika)} \qquad \Sigma_2(E) = -t_0 e^{(ika)}$$

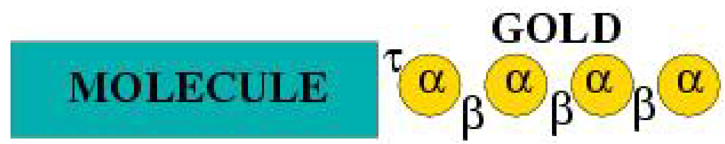
$$E = 2t_0(1 - \cos ka) \qquad \Gamma_{1,2} = i(\Sigma_{1,2} - \Sigma_{1,2}^{+}) = 2t_0 \sin ka$$

$$\hbar v(E) = 2at_0 \sin ka$$

$$G = [(E + i0^{+})I - H - \Sigma_1 - \Sigma_2]^{-1} = [i2t_0 \sin ka - (U_0 / a)]^{-1}$$

$$T(E) = Trace(\Gamma_1 G \Gamma_2 G^{+}) = \frac{\hbar v(E)^2}{\hbar v(E)^2 + U_0^{\,2}}$$

Toy 1-D Contacts



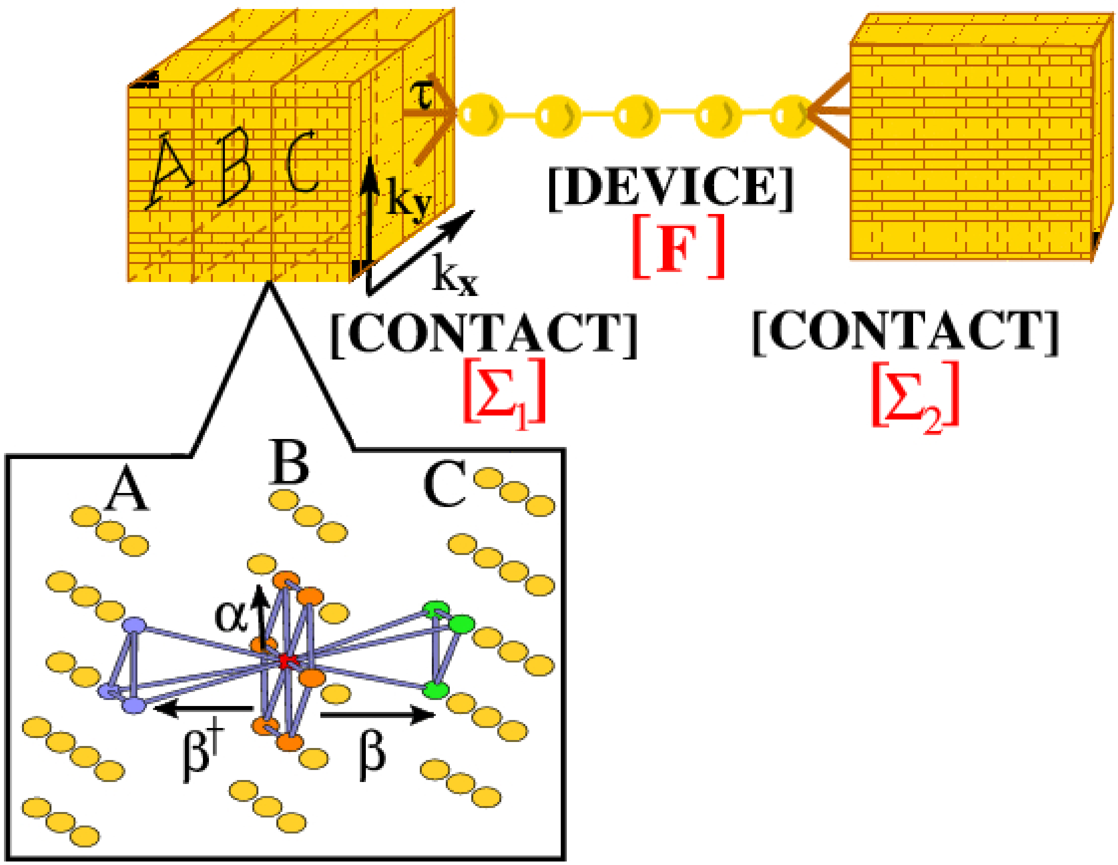
$$\Sigma = \tau g \tau^\dagger$$

$$G = \begin{bmatrix} \alpha & \beta & 0 & 0 & \dots \\ \beta^\dagger & \alpha & \beta & 0 & \dots \\ 0 & \beta^\dagger & \alpha & \beta & \dots \\ \dots & \dots & & & \end{bmatrix}^{-1} = \left[\begin{array}{c|cc} g & \dots & \dots \\ \hline & & \\ \dots & \dots & \\ \dots & \dots & \\ \dots & \dots & \end{array}\right]$$

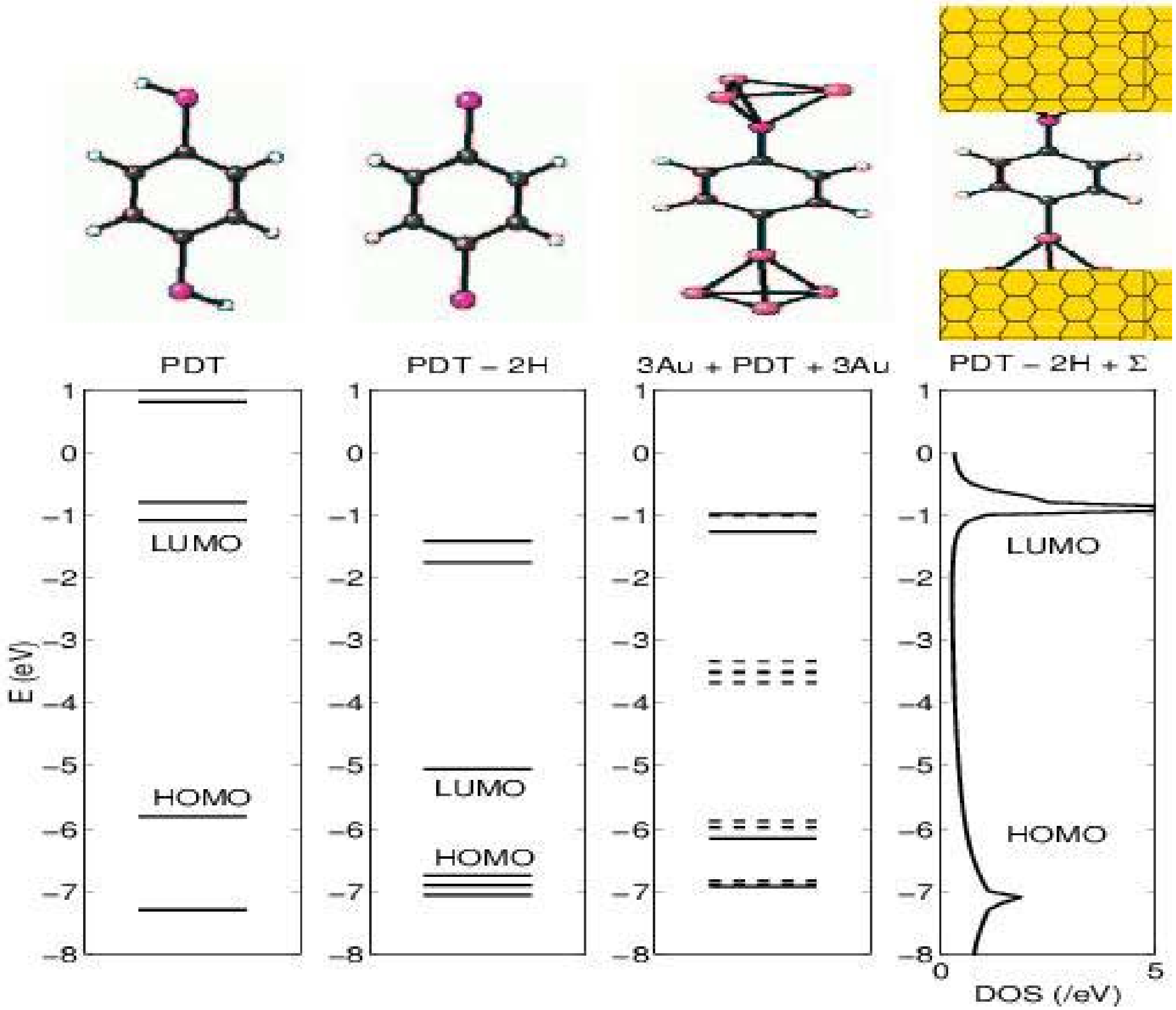
Solve for g iteratively from:

$$g = \left[\alpha - \beta g \beta^\dagger\right]^{-1}$$

Contacts in 3-D: K-space summation



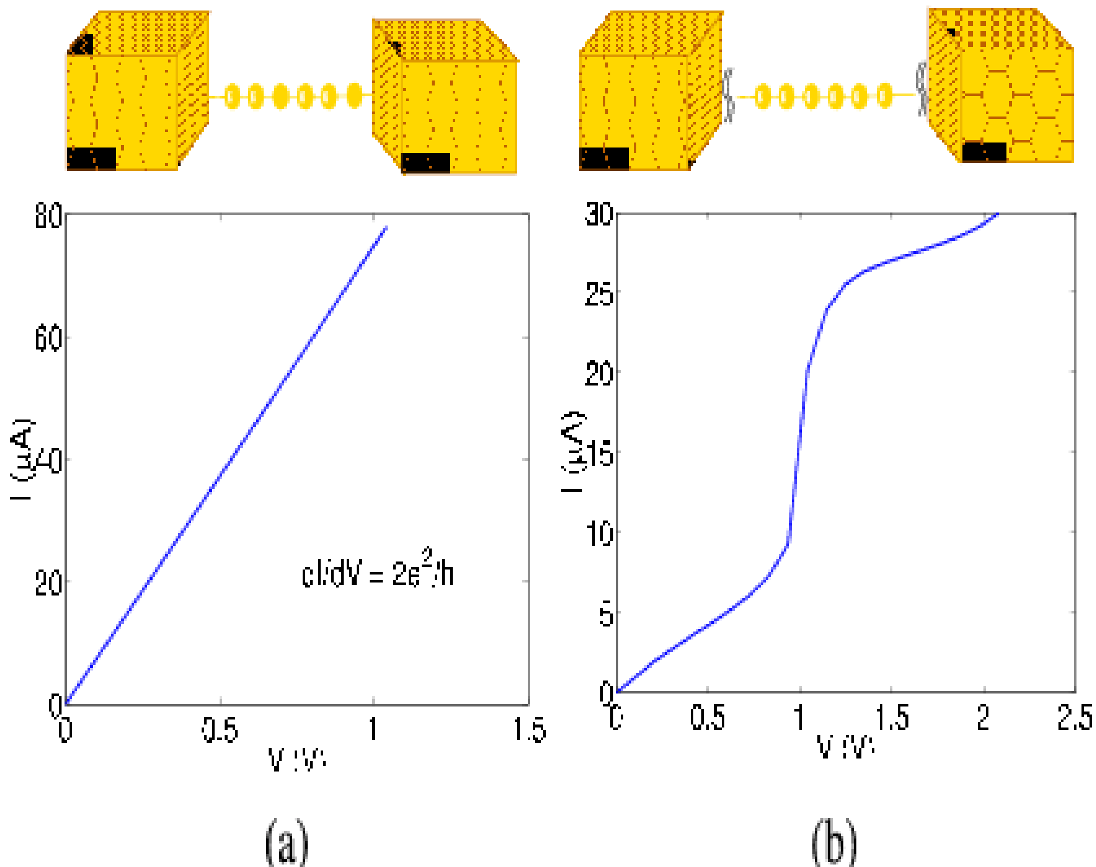
Self-Energy takes care of Chemistry



Methods of Calculation

- Toy
- Huckel
- Ab-initio

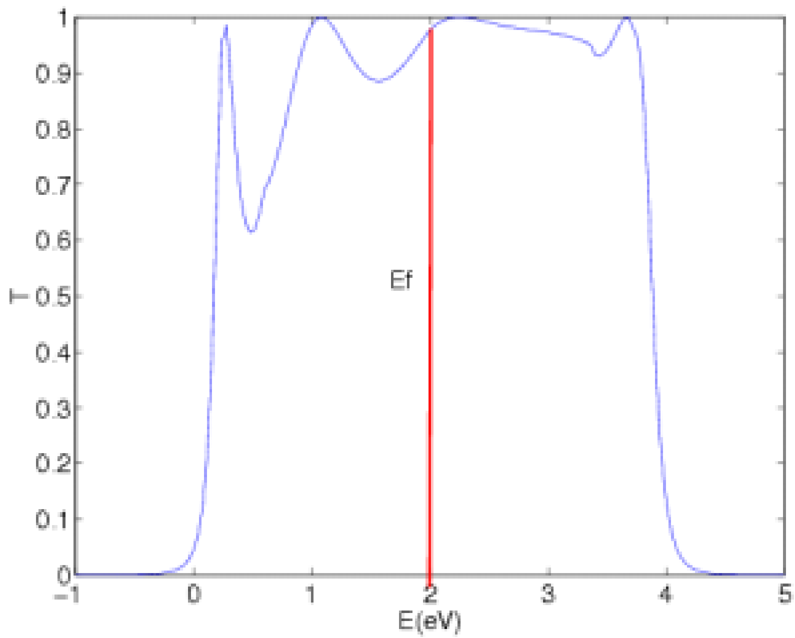
An Example: Quantum Point Contact I-V



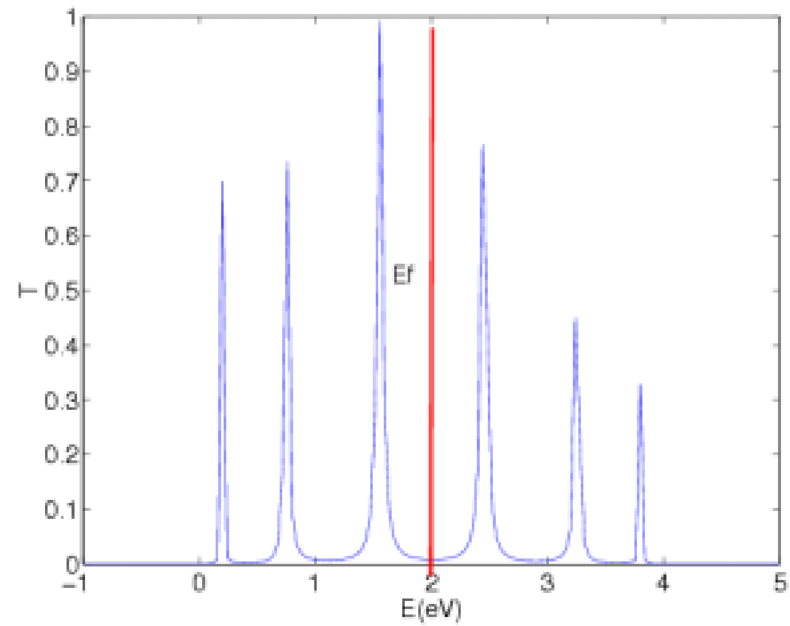
Strong Weak

Strong Coupling → quantized conductance ~ 77 μS

How does Transmission look like



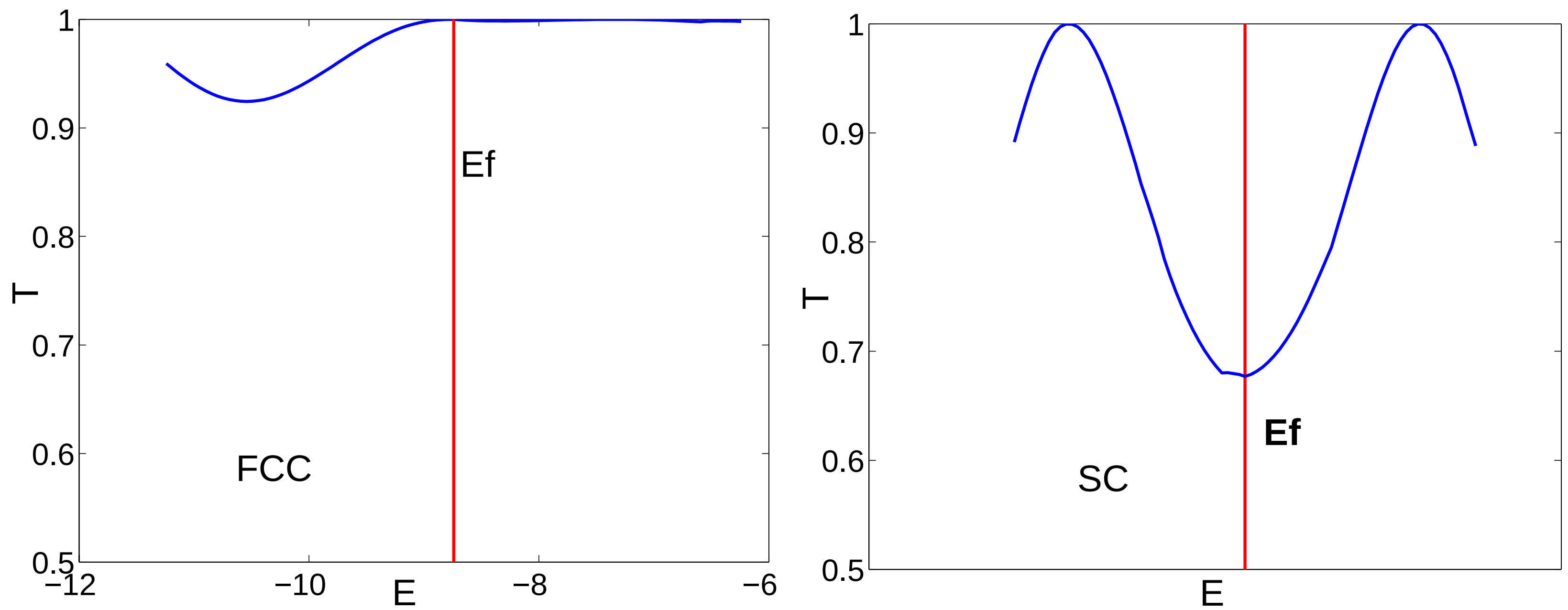
Strong



Weak

Transmission ~ 1 for a bias range > **quantum conductance**

Different Gold Contacts: FCC, Simple Cubic



Transmission differs for different gold contacts

Summary

- Contacts play crucial role in current conduction in small conductors
- Contact microstructure, bonding etc. has to be taken into account
- Green's function method provides a technique to incorporate effects of large contacts through self-energies
- Semi-infinite contacts can be replaced by self-energy matrices the same size as the device hamiltonian
- Self-energy has real and imaginary parts
- Imaginary part signifies finite lifetime of a carrier in an eigenstate