Fundamentals of Nanoelectronics

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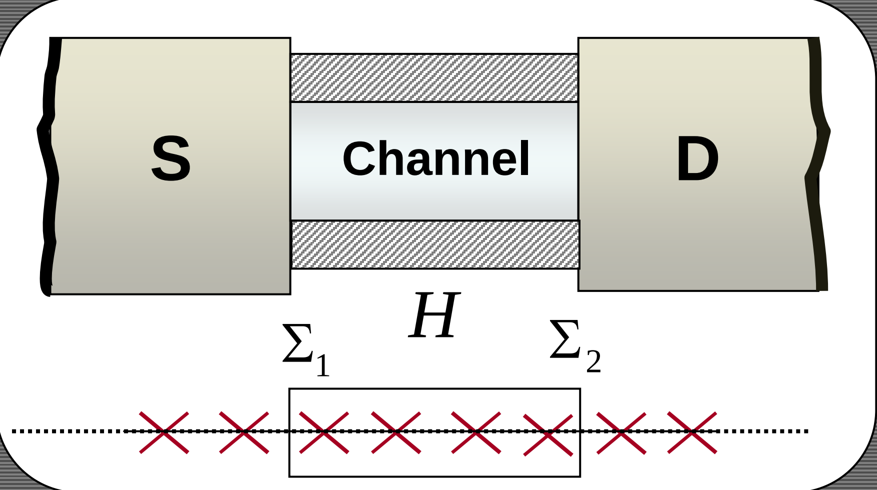
Lecture 33: Local Density Of States

Ref. Chapter: 8.2

Network for Computational Nanotechnology

NCN
nanoHUB
online simulations and more

Review



• We've learned in this course that we can describe the properties of any device a Hamiltonian H. For current flow however we also need to take into broadening which comes from the self energy functions Σ.

• For a one dimensional lead:

$$\Sigma_1 = \begin{bmatrix} -t_0 e^{ika} & & \\ & & \\ & & \end{bmatrix}$$

• Remember for closed systems we had:

$$[EI - H]\{\Psi\} = \{0\}$$

• But for open systems we got:

$$[EI - H - \Sigma]\{\Psi\} = \{S\}$$

• The important point to notice is that unlike H, Sigma is complex. The imaginary part indicates a finite lifetime and tells us how easily an electron can escape into the contact. The real part gives us broadening of the levels in the channel.

Lifetime and Broadening

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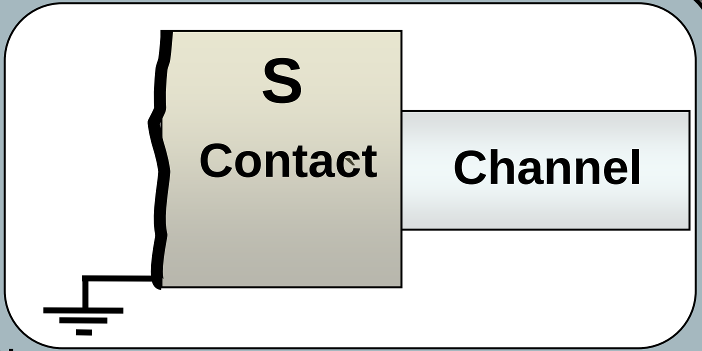
- Reminder: The electron density is the magnitude of psi^2 (see above). The expression for electron density shows the significance of the imaginary part of Σ . If there is not a coupling between the contact and channel the electron density remains constant. But if there is an imaginary part, the electron density has finite lifetime and it decays with time:



$$\tau = \gamma / \hbar$$

$$\left.\begin{aligned} \psi(t) &= \psi(0) e^{\frac{-i\varepsilon}{\hbar}t} e^{\frac{-i\Sigma}{\hbar}t} \\ \varepsilon' &= \varepsilon + \mathrm{Re}\,\Sigma \\ \gamma/2 &= -\,\mathrm{Im}\,\Sigma \end{aligned}\right\} \psi(t) = \psi(0) e^{\frac{-i\varepsilon'}{\hbar}t} e^{-\frac{\gamma}{2\hbar}t} \Rightarrow |\psi(t)|^2 = |\psi(0)|^2 e^{-t/\tau}$$

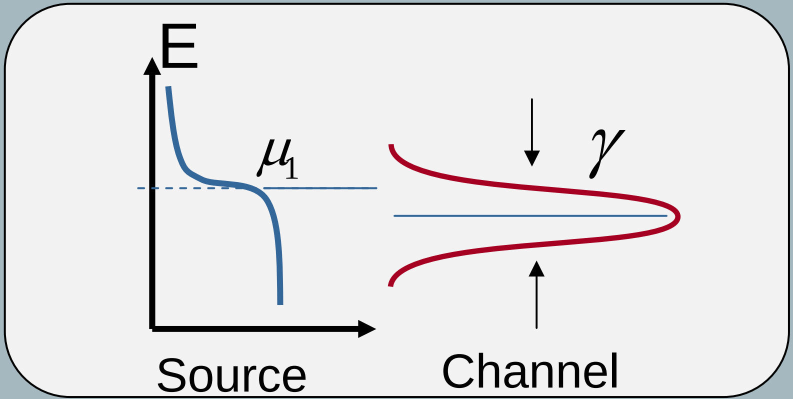
- There is also a broadening aspect to Σ which is related to the lifetime via uncertainty principle: The broadening is inversely proportional to the lifetime. We can calculate density of states as:

$$[EI - H - \Sigma]\{\Psi\} = \{S\} \quad \Rightarrow \{\psi\} = [G]\{S\}$$

$$[G] = [EI - H - \Sigma]^{-1}$$

$$A = i(G - G^{+})$$

$$\boxed{DOS = Trace(A)}$$

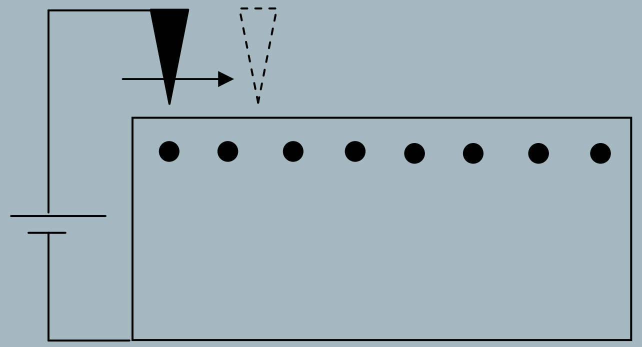


Why Local Density Of States ?

- The general definition of DOS is:

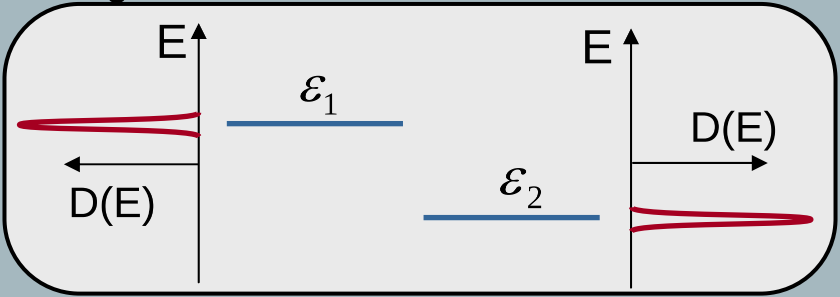
$$D(E) = \sum_{\alpha} \delta(E - \varepsilon_{\alpha})$$

- What the above equation tells us is the average number of states over the entire solid. However for nanostructures we are interested in local density of states. Notice that even for large solids the density of states changes on atomic scale. This is important because current depends on density of states. In the figure below when the tip is on top of atoms, density of states is higher and there is more current flow.



Spectral Function A(E)

• The next question is how to define a density of states with the property of being local?



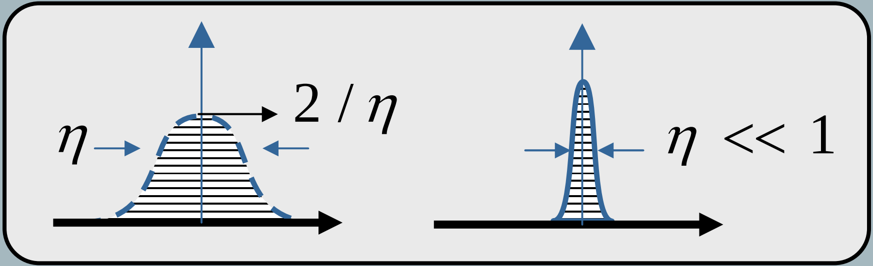
$$[H]=\begin{bmatrix}\varepsilon_1 & 0\\ 0 & \varepsilon_2\end{bmatrix}$$

$$A=2\pi\begin{bmatrix}\delta(E-\varepsilon_1) & 0\\ 0 & \delta(E-\varepsilon_2)\end{bmatrix}$$

• In general we are interested in the coupling between the levels. Before going about it, let's introduce a new definition for delta function.

$$2\pi\delta(x)=i\left\{\frac{1}{x+i\eta}-\frac{1}{x-i\eta}\right\},\ \eta\equiv 0^+$$

$$\Rightarrow 2\pi\delta(x)=\frac{2\eta}{x^2+\eta^2}$$



• G and A can be written as:

$$G=\begin{bmatrix}(E+i\eta)-\varepsilon_1 & 0\\ 0 & (E+i\eta)-\varepsilon_2\end{bmatrix}^{-1}$$

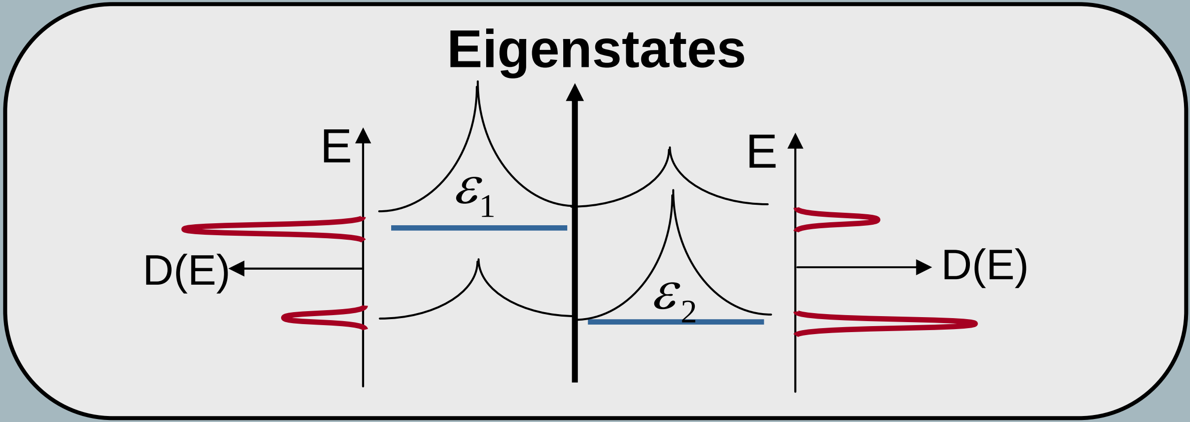
$$A(E)=i(G-G^+)\Rightarrow$$

$$A(E)=2\pi\begin{bmatrix}\delta(E-\varepsilon_1) & 0\\ 0 & \delta(E-\varepsilon_2)\end{bmatrix}$$

Coupling

- What happens to H if we have some coupling between levels? $[H] = \begin{bmatrix} \varepsilon_1 & \tau \\ \tau^+ & \varepsilon_2 \end{bmatrix}$
- G and A can be written as: $G = \left[(E + i\eta)I - H\right]^{-1}; A = i(G - G^+)$

Coupling of Two Levels



- One important nontrivial point is that after coupling, the height of Local Density Of States (LDOS) at each site (left and right) add up to 1.

Coupling TO The Contact

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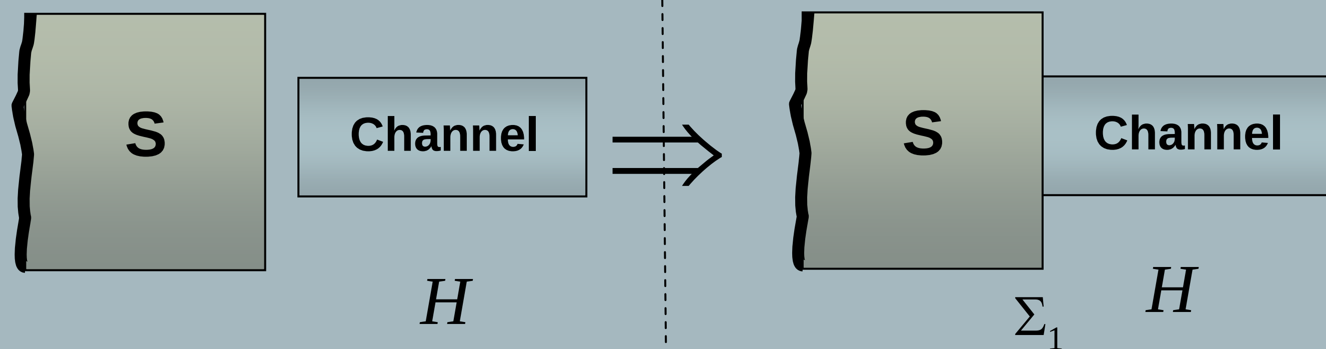
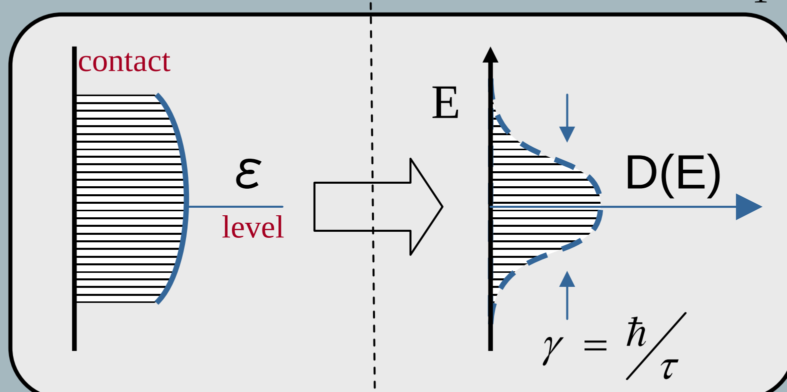
Before coupling $\Rightarrow$ After coupling





$$[H]=\begin{bmatrix}\varepsilon & & \\ & \varepsilon_1 & \\ & & \ddots\end{bmatrix} \Rightarrow [H]=\begin{bmatrix}\varepsilon & \tau_1 & \cdots \\ & \varepsilon_1 & \\ & & \ddots\end{bmatrix}$$