Quantum Transport:
Atom to Transistor

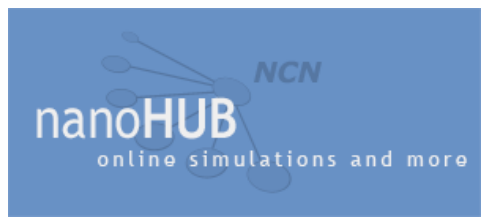
Prof. Supriyo Datta
ECE 659
Purdue University

03.26.2003

Lecture 27: Level Broadening: Self Energy

Ref. Chapter 8.2

Network for Computational Nanotechnology

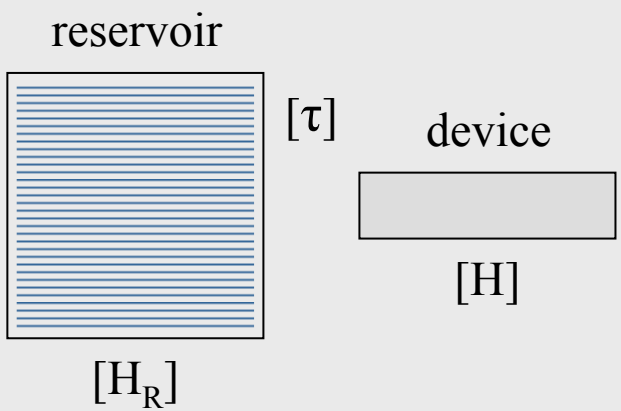


Working the System

00:00

• Recall, we often must deal with a device connected to a large reservoir. With different Hamiltonians for the device and reservoir associated by a coupling τ. We want to concentrate on the device.

Device and Reservoir



• The total Hamiltonian for the entire system (device and reservoir) is

$$\overline{H} = \begin{bmatrix} H & \tau \\ \tau & H_R \end{bmatrix}$$

• Last time we defined the concept of a spectral function, for the entire system it is given by

$$\overline{A} = 2\pi\delta\left(EI - \overline{H}\right)$$

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

$$= i\left[\overline{G} - \overline{G}^+\right]$$

Spectral Function

• Expanded out, the system spectral function is

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

We are only interested in calculating A, that part of the matrix which gives the local density of states in the device. Fortunately using Green's functions we can calculate A without dealing with the entire matrix Ā.

• One more comment about the spectral function. Don't forget it is given by

$$\overline{A} = 2\pi\delta(EI - \overline{H}), \text{ where}$$

$$2\pi\delta(x) = i\left\{\frac{1}{x + i0^+} - \frac{1}{x - i0^+}\right\}$$

• In general, any function of a matrix is calculated by diagonalizing the matrix, then taking the function of the diagonal elements and transforming back

Green's Function

06:20

• Later we will consider the physical meaning of the Green's function, today we will concentrate on evaluating the device Green's function.

• So, for the entire system we have a Green's function of the form

$$\overline{G} = \begin{bmatrix} \left(E + i0^+\right)I - H & -\tau \\ -\tau^+ & \left(E + i0^+\right)I - H_R \end{bmatrix}^{-1}$$

Note: the above formalism requires inversion of a very large matrix. If the device were not connected to the reservoir we would have τ=0 and the process would be much simpler

• Fortunately, to calculate device properties we need only the device Green's function G. We can get G by partitioning the matrix

• An example of matrix partitioning:

Given, $\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1}$

$$\therefore \begin{bmatrix} A & B \\ C & D \end{bmatrix}\begin{bmatrix} a & b \\ c & d \end{bmatrix} = I$$

Self Energy from Green's Function

14:20

$$\therefore \begin{bmatrix} A & B \\ C & D \end{bmatrix}\begin{bmatrix} a & b \\ c & d \end{bmatrix} = I \Rightarrow \left.\begin{matrix} Aa+Bc=I \\ Ca+Dc=0 \Rightarrow c=-D^{-1}Ca \end{matrix}\right\} Aa-BD^{-1}Ca=I \Rightarrow a=\left(A-BD^{-1}C\right)^{-1}$$

- We had:

$$\overline{G}=\begin{bmatrix} \left(E+i0^{+}\right)I-H & -\tau \\ -\tau^{+} & \left(E+i0^{+}\right)I-H_R \end{bmatrix}^{-1}=\begin{bmatrix} G & G_{dR} \\ G_{Rd} & G_{RR} \end{bmatrix}$$

- For the device Green's function we may apply this logic to get

$$G=\left[\left[\left(E+i0^{+}\right)I-H\right]-\Sigma\right]^{-1}, \text{where } \Sigma=\tau\left[\left(E+i0^{+}\right)I-H_R\right]^{-1}\tau^{+}=\tau G_R\tau^{+}$$

- Note, the size of Σ will be the same as that of the device since

$$\left.\begin{matrix} [\tau\ ]: (d \times R) \\ [G\ ]: (R \times R) \\ [\tau^{+}]: (R \times d) \end{matrix}\right\} \therefore \quad [\tau\, G_R\, \tau^{+}]: d \times d$$

- Why do we want G for the device? Remember, the spectral function for the device is $A = i\,[G\text{-}G^{+}]$ from which the local density of states and the density matrix may be calculated

Self Energy Matrix

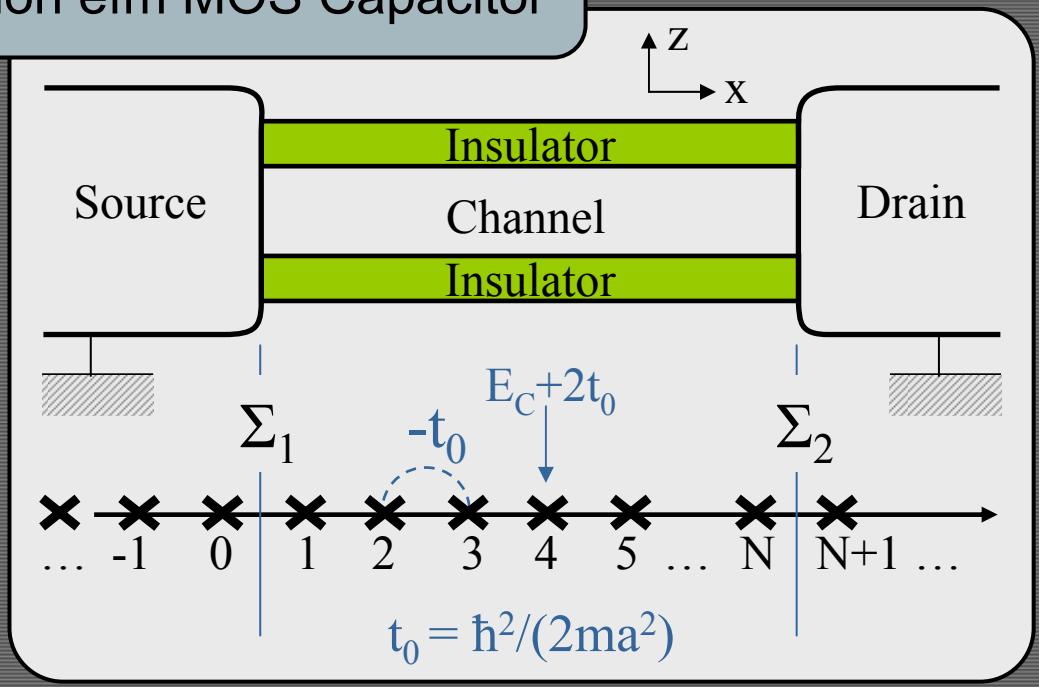
22:30

• How do we evaluate Σ given that G_R might be a million x million in size? The key is that we don't need the entire matrix G_R, but only that portion which has direct coupling to the device!

• To illustrate this process, let's look at an example, namely a 1-D effective mass model of our 1-D capacitor

• We want to find electron density in the channel or simply $A = i\,[G\text{-}G^{+}]$. Previously, periodic boundary conditions were assumed, that was incorrect, we can now treat open boundary conditions.

x-Direction efm MOS Capacitor



MOS Capacitor Example

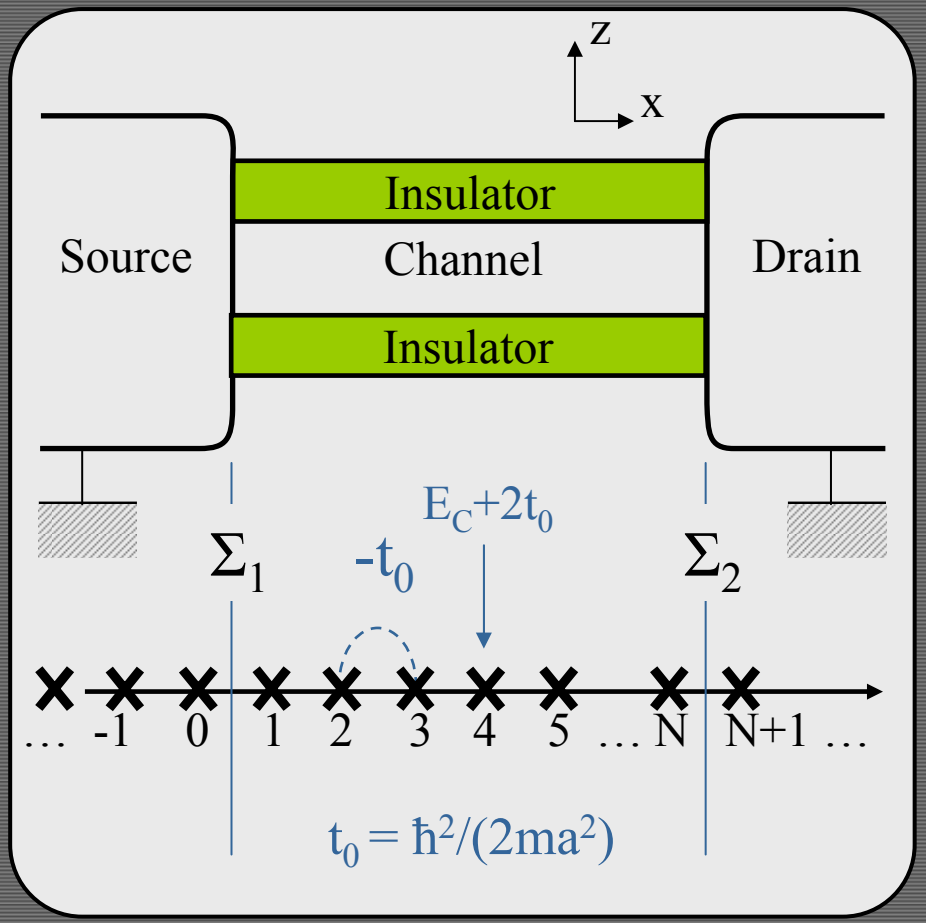
27:30

- So, how do we calculate Σ_1 and Σ_2, given $\sum = \tau G_R \tau^+$ since the left and right side are basically the same, let's concentrate on the left side
- First look at the coupling matrix, for this 1-D example it is

$$\tau_1 = \begin{matrix} d \\ \downarrow \end{matrix} \overset{R \rightarrow}{\begin{bmatrix} -t_0 & 0 & \cdots \\ 0 & 0 & \\ \vdots & & \ddots \end{bmatrix}}$$

Note: Only one point is connected, therefore all other points are zero

x-Direction efm MOS Capacitor



MOS Capacitor Example

• Element by element the self-energy matrix is

$$\Sigma_{mn} = (\tau_{ma})(G_R)_{a,b}(\tau^{+}_{b,n})$$

• Thus, Σ_1 has only one non-zero term at

$$(\Sigma_1)_{11} = t_0^2 G_R(0,0)$$

Importantly, we see that the only useful term in G_R is $G_R(0,0)$ which is referred to as the surface Green's function

• What is $G_R(0,0)$? First we'll state the answer and then justify,

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

where k is related to energy by the dispersion relation in the 1-D wire, that is

$$E = 2t_0(1 - \cos ka)$$

Hence, Σ is energy dependent.

• Side comment: Σ is not Hermitian since its diagonal elements are not real. Also, one can view the imaginary part of Σ in the eigenvalue basis as the lifetime of a state

Surface Green's Function

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

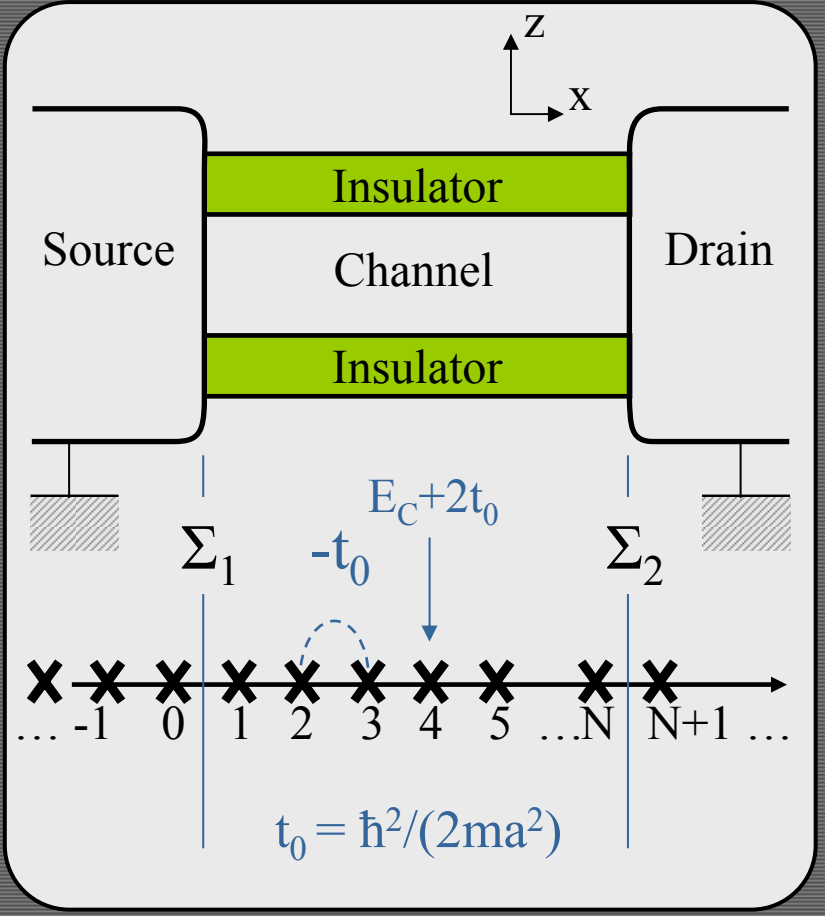
given, $G_R = \left[\left(E + i0^+\right)I - H_R\right]^{-1}$

$$\therefore G_R = \begin{bmatrix} E+i0^+ - E_C - 2t_0 & +t_0 & \cdots \\ +t_0 & E+i0^+ - E_C - 2t_0 & \\ \vdots & & \ddots \end{bmatrix}^{-1}$$

↑ tridiagonal

and $G_R^{-1} G_R = I$

x-Direction efm MOS Capacitor



Surface Green's Function

- Thus

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

multiplying through and equating both sides

$$\left[\left(E+i0^+\right)-E_C-2t_0\right]G_R(0,0)+t_0G_R(-1,0)=1 \quad (1)$$

to

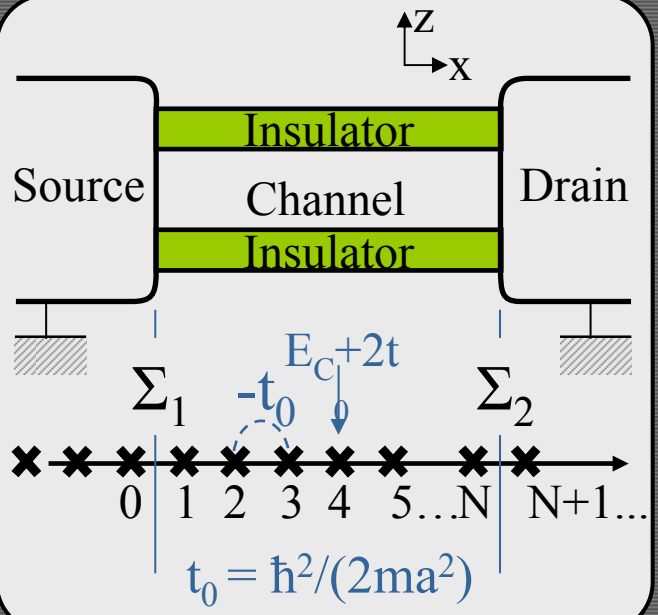
$$t_0G_R(0,0)+\left[\left(E+i0^+\right)-E_C-2t_0\right]G_R(-1,0)+t_0G_R(-2,0)=0 \quad (2)$$

or more generally to

$$t_0G_R(n+1,0)+\left[\left(E+i0^+\right)-E_C-2t_0\right]G_R(n,0)+t_0G_R(n-1,0)=0$$

for n<0

x-Direction efm MOS Capacitor



- Because this is periodic we may apply the ansatz

$$G_R(n,0)=G_R(0,0)e^{-inka}$$

Surface Green's Function

• Substituting the ansatz into ②

$$G_R(n,0) = G_R(0,0)e^{-inka}$$

we get

$$t_0 e^{ika} + \left(E + i0^+\right) - E_C - 2t_0 + t_0 e^{-ika} = 0$$

or

$$\left(E + i0^+\right) = E_C + 2t_0\left(1 - \cos ka\right) \text{ ③}$$

For the first equation, ①, substitute

$$G_R(-1,0) = G_R(0,0)e^{+ika}$$

$$\therefore G_R(0,0) = \frac{1}{\left(E + i0^+\right) - E_C - 2t_0 + t_0 e^{+ika}}$$

and now substitute ③ to get

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

• From $G_R(0,0)$ we may calculate Σ_1 and similarly Σ_2, which allows us to calculate G, A, and finally ρ

• Next Lecture:
Discuss the physical meaning of the Green's Function