Quantum Transport:
Atom to Transistor

Prof. Supriyo Datta
ECE 659
Purdue University

04.05.2004

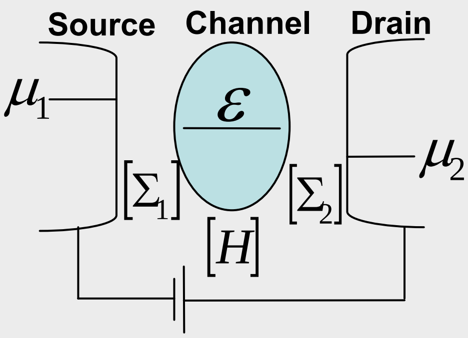
Lecture 30: Coherent Transport: Overview
Ref. Chapter 9.1

Network for Computational Nanotechnology

NCN nanoHUB online simulations and more

One Level Device

00:00



- The question is how to calculate the number of electrons inside the device and the current that flows through it. (This is a non-equilibrium problem i.e. two different Fermi levels.)
- At the beginning of the course the current and the electron density was obtained for a small one level device.

- In general, instead of a single level ε, the device is described by a Hamiltonian matrix whose eigenvalues give the energy levels $\varepsilon \rightarrow [H]$

Recap on the one level Device

$$I_1 = -\frac{q}{\hbar}\gamma_1(f_1 - N) \qquad I_2 = -\frac{q}{\hbar}\gamma_2(f_2 - N)$$

- Equating the two currents (in steady state) will give us the number of electrons N.

$$N = \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$$

- Substituting N back into either equation of I_1 or I_2 will give the current through the device. $I = -\frac{q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2}(f_1 - f_2)$
- After coupling, the discrete state (delta function) will be broadened according to the Lorentzian function.

Lorentzian Distribution

• Lorentzian function is defined as:

$$D_\varepsilon(E) = \frac{\gamma/2\pi}{(E-\varepsilon)^2 + \left(\gamma/2\right)^2} \qquad (\gamma = \gamma_1 + \gamma_2)$$

• And it can be incorporated in the current equations by setting up an integral over the energy.

• Equations of I_1 and I_2 now become:

$$I_1 = -\frac{q}{\hbar}\int dE\,\gamma_1\left(D_\varepsilon(E) f_1 - n(E)\right)$$

$$I_2 = -\frac{q}{\hbar}\int dE\,\gamma_2\left(D_\varepsilon(E) f_2 - n(E)\right)$$

• We now have a distribution of levels instead of just one level and to get the total current (if the levels are independent) we can just sum all currents; hence integrating over energy.

• N Becomes: $N = \int dE D_\varepsilon(E) \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$

• Finally we have:

$$I = -\frac{q}{\hbar}\int dE D_\varepsilon(E) \frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2}(f_1 - f_2)$$

$D_\varepsilon(E) \frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2} \rightarrow T(E)/2\pi$

• This equation tells us that the current flows due to the difference of agenda between f1 and f2.

• What we've done thus far is a review of first couple of weeks. In general our quantities like ε or γ become matrices.
$(\varepsilon \rightarrow [H], \gamma \rightarrow [\Sigma]$,etc)

• The next step is to derive the matrix equations of the number of electrons and current.

Matrix Equations

- As we have discussed before, a useful concept is that of Green's Function:

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

- Having Green's function, one can calculate the density of states; namely the spectral function A which is defined as: $A = i\left(G - G^{+}\right)$

We now define the quantity Γ, which is physically the imaginary part of Σ:

$$\Gamma_1 = i(\Sigma_1 - \Sigma_1^{+}) \quad \Gamma = i(\Sigma - \Sigma^{+})$$

$$\Gamma_2 = i(\Sigma_2 - \Sigma_2^{+})$$

- The matrix equation for N is:

$$N = Trace \int dE \left(\left[A_1\right] f_1 + \left[A_2\right] f_2\right)$$

- Where $A_1 = G\Gamma_1 G^{+}$, $A_2 = G\Gamma_2 G^{+}$
- We can describe Transmission as:

$$T(E) = Trace \; (\Gamma_1 G \Gamma_2 G^{+})$$

Note that $A = A_1 + A_2$

And $\left(\left[A_1\right] f_1 + \left[A_2\right] f_2\right) = G^{n}$

- Current at the source or the drain contact:

$$I_i = -\frac{q}{\hbar} \int dE (Trace(\Gamma_i A) f_i - Trace(\Gamma_i G^{n})$$

- Net Current through the device:

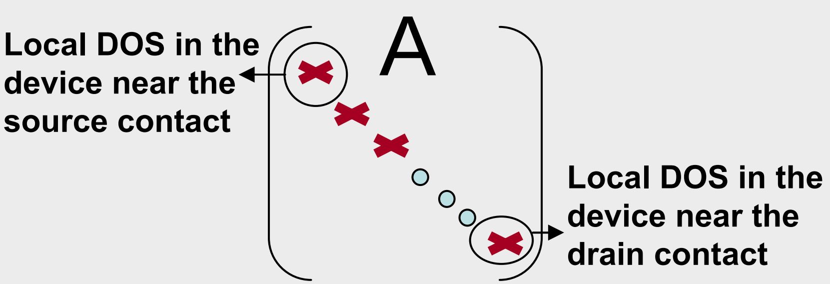
$$I = -\frac{q}{\hbar} \int dE Trace(\Gamma_1 G \Gamma_2 G^{+})(f_1 - f_2)$$

Summary of Results

26:27

- $G = \left(EI - H - \Sigma\right)^{-1} \qquad (\Sigma = \Sigma_1 + \Sigma_2)$
- $A = i\left(G - G^+\right) = A_1 + A_2$
- $\Gamma_1 = i(\Sigma_1 - \Sigma_1^+) \qquad \Gamma_2 = i(\Sigma_2 - \Sigma_2^+)$

  $\Gamma = i(\Sigma - \Sigma^+)$
- $A_1 = G\Gamma_1 G^+ \quad A_2 = G\Gamma_2 G^+$
- $T(E) = Trace\,(\Gamma_1 G \Gamma_2 G^+)$
- $G^n = ([A_1] f_1 + [A_2] f_2)$



Recap and Overview

- All various quantities that were discussed at the beginning of the course have corresponding matrix versions.

- The diagonal elements of the matrix in its real space representation give the value of the quantity at various points.

- For example consider the spectral function A. Its diagonal elements represent the local density of states at different points.

Summary of Results

27:15

- $G = (EI - H - \Sigma)^{-1} \quad (\Sigma = \Sigma_1 + \Sigma_2)$
- $A = i(G - G^+) = A_1 + A_2$
- $\Gamma_1 = i(\Sigma_1 - \Sigma_1^+) \quad \Gamma_2 = i(\Sigma_2 - \Sigma_2^+)$

  $\Gamma = i(\Sigma - \Sigma^+)$
- $A_1 = G\Gamma_1 G^+ \quad A_2 = G\Gamma_2 G^+$
- $T(E) = Trace\,(\Gamma_1 G \Gamma_2 G^+)$
- $G^n = ([A_1]f_1 + [A_2]f_2)$

- When the DOS (A) is connected to the reservoirs, it can be broken into 2 parts, A1 and A2. (A=A1+A2)
- Just like the case of one level model that a fraction gets filled according to f1 and a fraction according to f2, here A1 gets filled according to f1 and A2 gets filled according to f2. G^n (electron density) tells us what's filled and can be calculated by summing A1f1 with A2f2.
- The important point is that these equations can be used to solve any type of complex problem to get the current passing through the device.
- Notice that the limiting case of the equations (where matrices become 1*1) will result in what we had for the one level model.

From matrix equations to one level model

$$H \Rightarrow [\varepsilon]$$

- H becomes a matrix with one entry. (Just one level ε)

$$\Sigma_1 \Rightarrow \left[\sigma_1 - \frac{i\gamma_1}{2}\right], \quad \Sigma_2 \Rightarrow \left[\sigma_2 - \frac{i\gamma_2}{2}\right] \Rightarrow \Sigma = \left[\sigma - \frac{i\gamma}{2}\right]$$

$$\gamma = \gamma_1 + \gamma_2, \quad \sigma = \sigma_1 + \sigma_2$$

- Σ has a real part which is written as σ and an imaginary part written as $\frac{i\gamma}{2}$.

$$G = \frac{1}{E - \varepsilon - \sigma + \frac{i\gamma}{2}}$$

- Considering G physically, the presence of σ shifts the level up or down and $\frac{i\gamma}{2}$ has to do with the level broadening or the escape rate out of the device. (Lifetime of the particle)

$$A = i\left[\frac{1}{E - \varepsilon - \sigma + \frac{i\gamma}{2}} - \frac{1}{E - \varepsilon - \sigma - \frac{i\gamma}{2}}\right] = \frac{\gamma}{(E-\varepsilon-\sigma)^2 + (\gamma/2)^2}$$

From matrix equations to one level model

- But what are A1 & A2 and do they add up to A?

$$A_i = G\gamma_i G^+ = \frac{\gamma_i}{(E-\varepsilon-\sigma)^2 + (\gamma/2)^2}$$

$$A = A_1 + A_2 = G\gamma_1 G^+ + G\gamma_2 G^+ = \frac{\gamma}{(E-\varepsilon-\sigma)^2 + (\gamma/2)^2}$$

$$(A = 2\pi D(E))$$

- Transmission $T = \gamma_1 G \gamma_2 G^+ = \dfrac{\gamma_1\gamma_2}{(E-\varepsilon-\sigma)^2 + (\gamma/2)^2}$

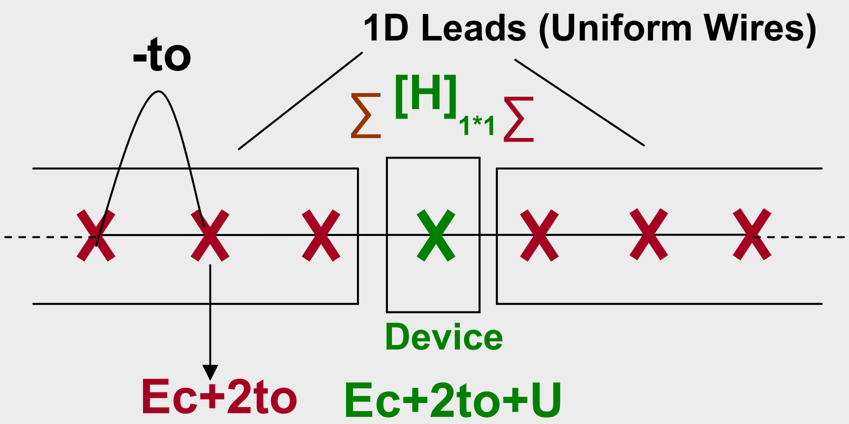
- As it can be seen from these derivations, matrix equations do in fact reduce to the equations that we had for the one level model in their limiting case in which they become one by one matrices.
- One can think of deriving general matrix equations from the 1X1 case by thinking that both [H] and [∑] are diagonal matrices and individual diagonal entries are contributing to the current INDEPENDENTLY. It then makes sense to sum up all these contributions in order to get the net current. But this is something we cannot do in general, because [H] and [∑] cannot be diagonalized simultaneously.

[H] & [Σ]

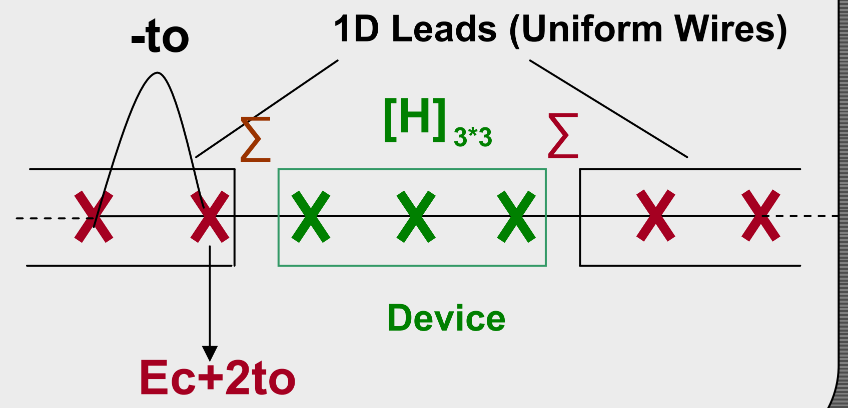
45:25

Example

Small One Level Device



Three Level Device



$$\Sigma_1 = \begin{pmatrix} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad [H]_{3*3} = \begin{pmatrix} Ec+2to+U_1 & X & 0 \\ X & Ec+2to+U_2 & X \\ 0 & X & Ec+2to+U_3 \end{pmatrix} \qquad \Sigma_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -t_0 e^{ika} \end{pmatrix}$$

[H] & [∑]: Simultaneous Diagonalization

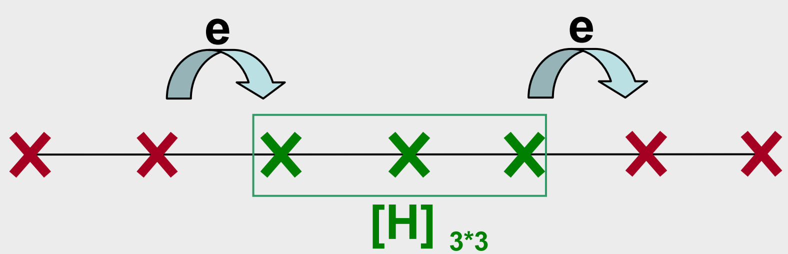
48:45

$$\Sigma_1 = \begin{pmatrix} -t_0 e^{ika} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad [H]_{3*3} = \begin{pmatrix} Ec+2to+U_1 & \times & 0 \\ \times & Ec+2to+U_2 & \times \\ 0 & \times & Ec+2to+U_3 \end{pmatrix} \qquad \Sigma_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -t_0 e^{ika} \end{pmatrix}$$

- Physically there are three levels (in the device) that are connected to one another which result in the off diagonal terms in the Hamiltonian matrix. On the other hand the leads into which electrons can empty are connected to point 1 on the left and to point 3 on the right. This is shown by the escape rates in the ∑1 and ∑2 matrices.

- In the present representation ∑1 and ∑2 are diagonal while [H] is not. One can derive the representation in which [H] is diagonalized but then ∑1 and ∑2 wouldn't be diagonal any more.

[H] & [∑] Different Representations

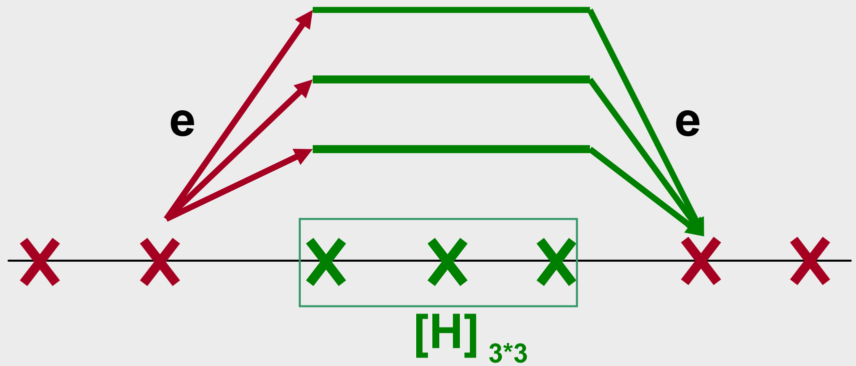


[H] with representation

(With off diagonal terms)

Real Space Representation

Eigen State Representation



Diagonalized [H]

- When [H] is diagonalized, the incoming electron will not just go in one level, but it will go in all three levels in fractions. It is similar when the electron exits the device. It will exit from all three levels. This is reflected by the fact that ∑1 and ∑2 are not diagonal and have off diagonal entries.

- Notice that all of this is taken care of, with using the matrix equations.