Quantum Transport:
Atom to Transistor

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Lecture 38: Incoherent Transport
Ref. Chapter 9.4

Network for Computational Nanotechnology

nanoHUB online simulations and more

Emission/ Absorption

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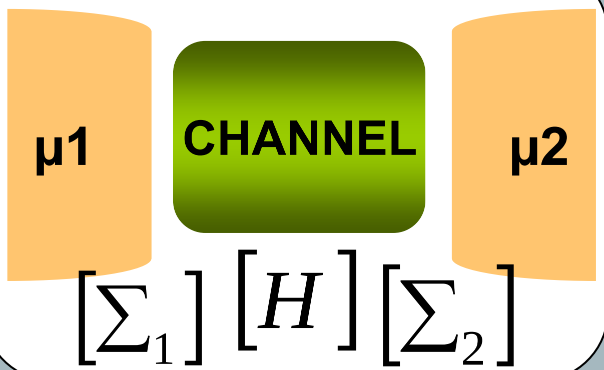


$$\Gamma_j = i\left(\Sigma_j - \Sigma_j^+\right)$$

$$\Sigma = \Sigma_1 + \Sigma_2$$

$$\Gamma = \Gamma_1 + \Gamma_2$$

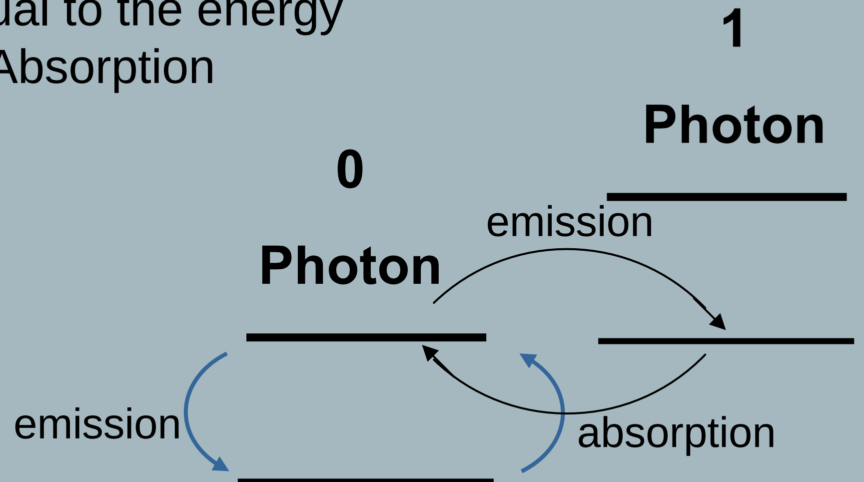
$$G = \left(EI - H - \Sigma\right)^{-1}$$

$$A = i\left(G - G^+\right)$$

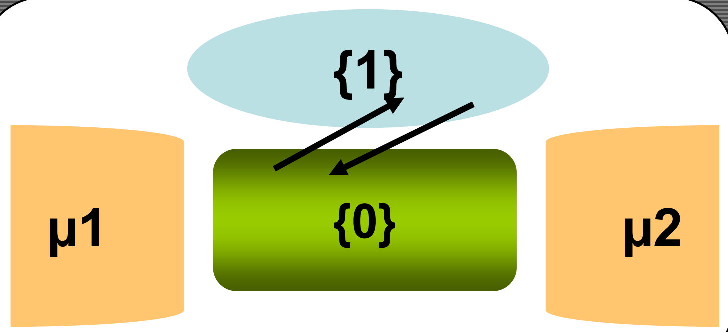
Today we want to discuss how to incorporate the effects of Inelastic scattering into the description of current flow.

- For long devices, one needs to include the effect of incoherent scattering mechanism.
- Conceptually one can think of them as:

Emission energy is NOT equal to the energy of Absorption



Scattering viewed as a contact



• Consider 0 degrees Kelvin. There is no phonons, but the electron can give rise to phonons and might get scattered because it can give rise to phonons. Now this is incoherent scattering process where the electron looses energy by passing through the device and changes the state of the system.

• A good way of thinking about the incoherent process is to think of an additional contact. In this case the channel would be at equilibrium where no phonons are generated in it; instead they are being generated in this additional contact.

• One main difference between this virtual contact and a real one is that the real contacts are in equilibrium and do have a defined Fermi function. Such is NOT the case for this additional contact because the channel is not in equilibrium. But the simplest description is to assume a potential μ_S and impose the condition that there must not be a net current between the channel and this additional contact.

• This also helps to describe the difference between coherent and incoherent processes.

Coherent vs. Incoherent Transport

- Question: What is the difference between coherent and incoherent scattering?
- Answer: Coherent transport is one for which electron passes through the device and NOTHING else gets affected by it. i.e. no phonons are generated. It is like going through a rigid body *without* changing anything or any jiggling in the body. Impurity scattering is an example where the positive impurity ion does not vibrate or get deflected when it deflects and scatters the electron. On the contrary incoherent processes are in a way that the surrounding does get affected by the transport of electron. In other words the state of the system changes as the result of transport.

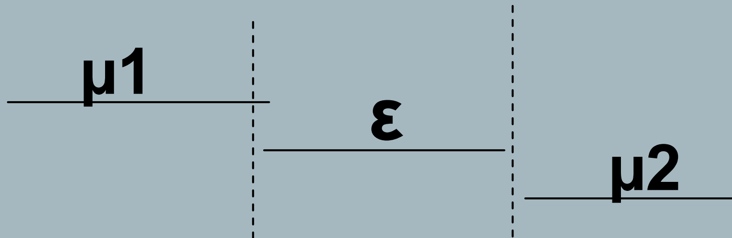
- Why are we considering incoherent transport? Because as soon as one gets to large devices, such processes must be taken into account for correct results. For example without considering it resistance would be changing exponentially with length for a piece of long device which would be totally wrong.
- The first thing we can do is to investigate current flow through the device having multiple contacts.
- In this course we've described the current for a two contact device like the following: $I_j(E) = \int dE\, \tilde{I}_j(E)$

$$\tilde{I}_j(E) = Trace\left[\Gamma_j A\right] f_j - Trace\left[\Gamma_j G^n\right]$$

- This could easily be understood for a one-level device discussed on the next page.

Current in terms of Transmission

- Current for one level Device:



$$I_1 = \int dE\, D(E) \frac{\gamma_1}{\hbar}\left(f_1 - N\right)$$

$$I_2 = \int dE\, D(E) \frac{\gamma_2}{\hbar}\left(f_2 - N\right)$$

$$\tilde{I}_i(E) = Trace\left[\Gamma_i A\right] f_i - Trace\left[\Gamma_i G^n\right]$$

- Another way of writing current is to substitute for the expression of G^n to put it in the form of transmission multiplied by the difference of the two Fermi functions.

$$\tilde{I}_i = \underbrace{Trace\left(\Gamma_i G \Gamma_g G^+\right)}_{\bar{T}(E)}\left(f_i - f_j\right)$$

- You can think of transmission as the probability at which electrons transmit through the device.
- Based on the concept of transmission, Buttiker introduced this relation for the current in multiple contact devices:

$$\tilde{I}_i = \sum_j \bar{T}_{ij}(E)\left(f_i - f_j\right)$$

Transmission in a Multi-Contact Device

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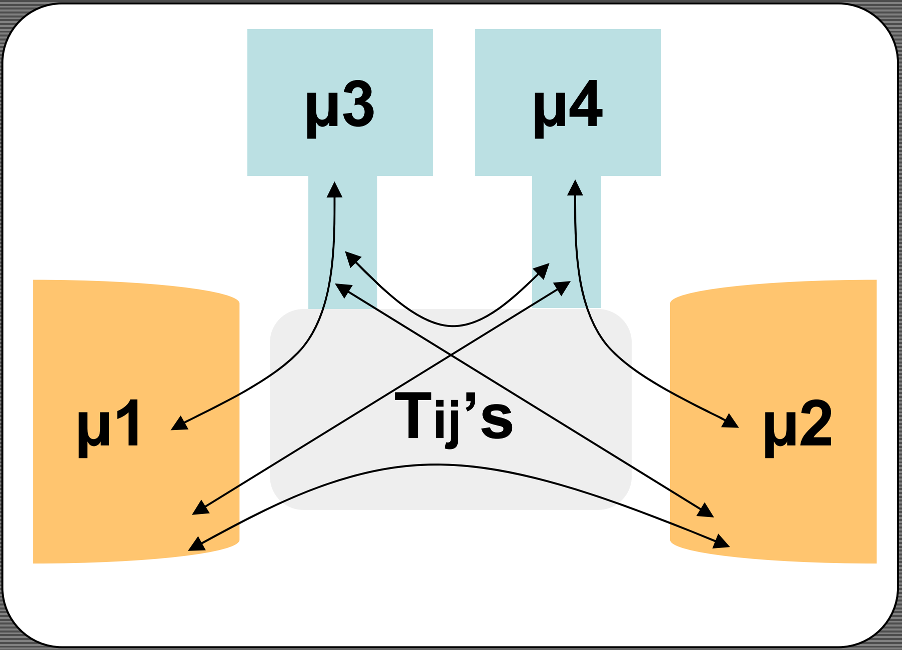


- For the four terminal structure you can define transmission between any two terminals. So in general:

$$\tilde{I}_i = \sum_j Trace\left(\Gamma_i G \Gamma_g G^+\right)\left(f_i - f_j\right)$$

- You can see that it works for our two contact device:

$$\tilde{I}_1 = \sum_j \bar{T}_{ij}(E)\left(f_1 - f_j\right)$$

$$= \bar{T}_{11}(E)(f_1 - f_1) + \bar{T}_{12}(f_1 - f_2) \Rightarrow$$

$$\tilde{I}_1 = \bar{T}(f_1 - f_2)$$

- The transmission for the 4 terminal device would become a 4 by 4 matrix:

$$\begin{array}{cc} & \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} & \left(\begin{array}{cccc} \quad & \quad & \quad & \quad \\ & & & \\ & & & \\ & & & \end{array}\right) \end{array}$$

Matrix method for current

• The current can then be written in the form of some matrix:

$$\tilde{I}_i = \sum_j Trace\left(\Gamma_i G \Gamma_g G^+\right)\left(f_i - f_j\right)$$

$$\begin{Bmatrix} \tilde{I}_1 \\ \tilde{I}_2 \\ \tilde{I}_3 \\ \hline \tilde{I}_4 \end{Bmatrix} \begin{matrix} \\ = \\ \mathbf{0} \\ \end{matrix} \left(\begin{array}{c|c} \quad & \quad \\ \hline \quad & \quad \end{array}\right) \begin{Bmatrix} f_1 \surd \\ f_2 \surd \\ f_3 \\ \hline f_4 \end{Bmatrix}$$

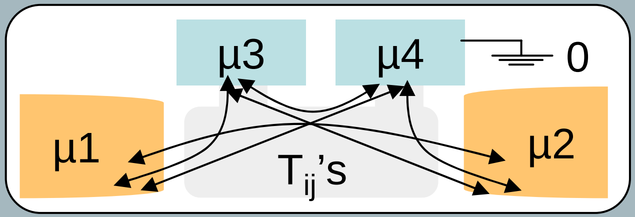
• The way this works is that we usually know the voltages at the four terminals which will give the Fermi functions. By knowing the transmission we can then calculate the current. How ever in our case, we don't know the voltages for the two probes (i.e. we don't know µ3 & µ4) because they are floating . In fact we want to measure these voltages.

• But note that the Transmission matrix relates the current vector to the Fermi function vectors; hence knowing any four quantities will give us the other four.

<u>A point on using matrix method to solve the equations</u>

• From linear algebra we know that in a system of linear equations, the ones that are dependent (i.e. can be written as linear combination of the others) can be eliminated. In fact they don't give us any new information that is not already in the others. This is indeed the case for our 4 terminal device.

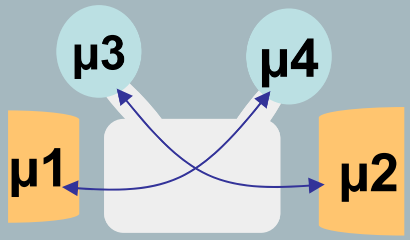
Virtual Contacts



• For example from Kirchoff's current law we know that the algebraic sum of all currents entering the channel must be 0. Same goes for voltages. So, conceptually one can eliminate one of the equations; or in other words one of the quantities can be set to 0. We'll set μ4 to 0 and solve for the rest of it.

• One important point is that if we keep all four equations, they won't be independent; hence the T-matrix will have no inverse and will be singular.

• This whole concept helps us to treat coherent transport through a multi terminal device. It has also helped people to understand the device better. For instance in mid 1980's, in some experiments, it was observed that by applying a voltage to contacts 1 and 2 in a small device, one would get negative resistance i.e. the probe that had to have rather higher voltage, actually had a smaller one. Physically, this happened because electrons could transport to contact 4 easier than 3 and hence contact 4's voltage was closer to contact 1 and contact 3's voltage was closer to contact 4's voltage. But Buttiker's equations can predict such behavior and give the right results.

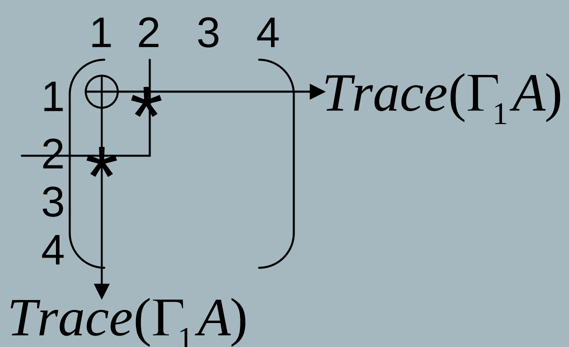


Towards Sum Rule

- Now if we use the expression

$$\bar{T}_{ij} = Trace\left(\Gamma_i G \Gamma_j G^+\right)$$

for transmission, we can prove an interesting result called the sum rule. Here is an illustration of what it is:

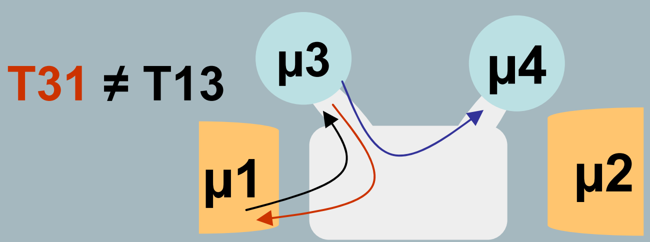


$$T_{12} = Trace\left(\Gamma_1 G \Gamma_2 G^+\right)$$

$$T_{21} = Trace\left(\Gamma_2 G \Gamma_1 G^+\right)$$

Is $T_{12} = T_{21}$**?**

- This is not true in general. For instance consider a device in a magnetic field and you can see this physically. When the electron enters the channel, its trajectory gets rotated and Transmission between two terminals is not necessarily reciprocal.



- So how do we prove the sum rule? The proof comes on the next page.

Proving The Sum Rule

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$$G=\left(EI-H-\Sigma\right)^{-1} \qquad \Gamma=\Gamma_1+\Gamma_2+\Gamma_3+\Gamma_4$$

$$\underbrace{A \equiv i\left(G-G^+\right)}_{\text{Definition}} = \underbrace{G\Gamma G^+ = G^+\Gamma G}_{\text{Can prove}}$$

$$T_{ij} = Trace\left(\Gamma_i G \Gamma_j G^+\right)$$

$$\begin{cases} \sum_j T_{ij} = \sum_j Trace\left(\Gamma_i G \Gamma_j G^+\right) = Trace\left(\Gamma_i \underbrace{G\Gamma G^+}_{\mathbf{A}}\right) \\ \sum_j T_{ji} = \sum_j Trace\left(\Gamma_j G \Gamma_i G^+\right) = Trace\left(\Gamma G \Gamma_i G^+\right) \end{cases}$$

$$\Rightarrow \begin{cases} \sum_j T_{ij} = Trace\left(\Gamma_i \underbrace{G^+\Gamma G}_{\mathbf{A}}\right) = Trace(\Gamma_i A) \\ \sum_j T_{ji} = Trace\left(\Gamma_i \overbrace{G\Gamma G^+}\right) = Trace(\Gamma_i A) \end{cases}$$

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Scattering as a virtual Contact

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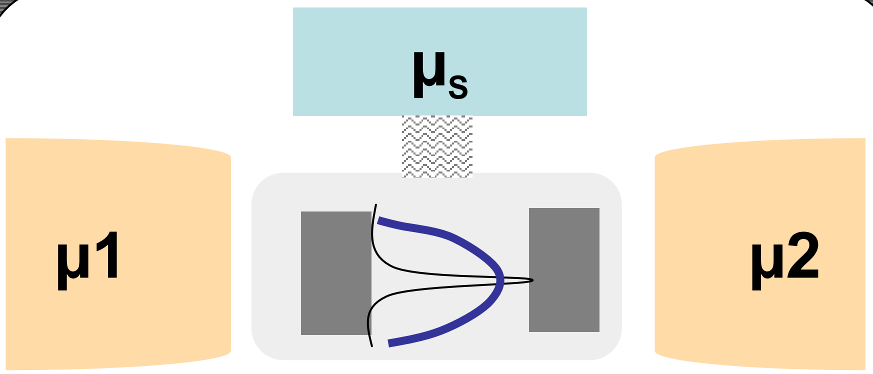

- The properties of this device is like the multi-terminal device discussed at the beginning of the lecture; namely it has a chemical potential μ_s which adjusts itself such that our relations are right and there is no net current across it.
- Our equations now become:

$$\Gamma = \Gamma_1 + \Gamma_2 + \Gamma_S$$

$$\Sigma = \Sigma_1 + \Sigma_2 + \Sigma_S$$

- For current we'll have the same expression:

$$\tilde{I}_i(E) = Trace\left[\Gamma_i A\right] f_i - Trace\left[\Gamma_i G^n\right]$$

- This virtual terminal is useful even when the scattering is not present. For example, in resonant tunneling devices having this contact will broaden the transmission which would have been very sharp without it therefore a very fine energy grid would have been necessary for the calculation of current whereas by including this virtual terminal and hence introducing scattering, we could use a much coarser energy grid.

In-scattering

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- To find the equation of current, let's start with the electron density:

$$G^n(E) = \left(G\Gamma_1 G^+\right) f_1 + \left(G\Gamma_2 G^+\right) f_2 + \left(G\Gamma_S G^+\right) f_S$$

- Putting it in compact form,

$$G^n = G\Sigma^{in} G^+$$

$$\Sigma^{in} = \Gamma_1 f_1 + \Gamma_2 f_2 + \cancel{\Gamma_S f_S}$$

$$\Sigma_S^{in}\left(E\right) = D_0 G^n\left(E\right)$$

- We modify this last equation to compensate for the fact that electrons are coming in from higher energy and emit a photon. So,

$$\Sigma_S^{in}\left(E\right) = D_0 G^n\left(E + \hbar\omega\right)$$

We also include absorption processes to get:

$$\Sigma_S^{in}\left(E\right) =$$

$$D_0 \times (N+1) G^n\left(E + \hbar\omega\right)$$

$$+ D_0 \times (N) G^n\left(E - \hbar\omega\right)$$