Quantum Transport:
Atom to Transistor

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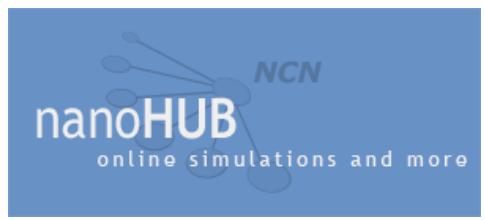
Lecture 32: Non-equilibrium Density Matrix

Ref. Chapter 9.2

Network for Computational Nanotechnology



Current Flow

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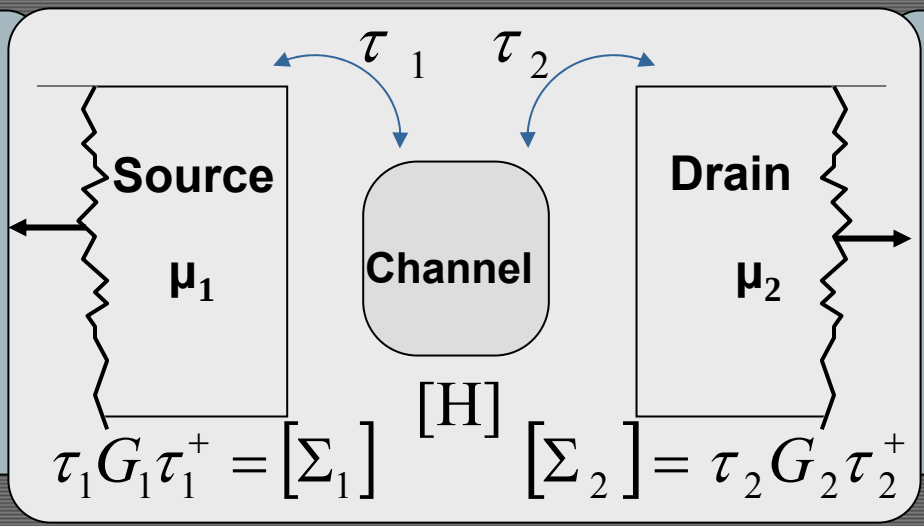
• **Reminder: We're discussing the current flow through the channel connected to the source and drain contacts with two different chemical potentials.**

• **Towards the beginning of the course we discussed this problem for a single level device and we derived the equations with common sense argument without much use of quantum mechanics.**

• Huge size; however the effect on the channel can be written using $\sum_1$ which has the same size as that of the channel.



• Huge size; however the effect on the channel can be written using $\sum_2$ which has the same size as that of the channel.

$$\left[EI - H_1 + i0^-\right]^{-1} = G_1$$

$$G_2 = \left[EI - H_2 + i0^+\right]^{-1}$$

Density Matrix; Current

$$[\rho] = \int \frac{dE}{2\pi} [G^n(E)]$$ want to derive

$$G^n = ([A_1]f_1 + [A_2]f_2)$$

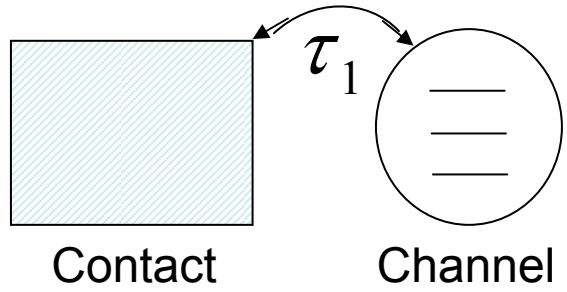
$$A_1 = G\Gamma_1 G^+ \qquad A_2 = G\Gamma_2 G^+$$

$$G = (EI - H - \Sigma_1 - \Sigma_2)^{-1}$$

$$I_i = \left(-\frac{q}{\hbar}\right)\int \frac{dE}{2\pi}\tilde{I}_i(E)$$ want to derive

$$\tilde{I}_i(E) = Trace(\Gamma_i A)f_1 - Trace(\Gamma_i G^n)$$

- Next, we want to derive G^n.



- Schrödinger Equation
- General Form $E\Psi = \overline{H}\Psi$
- Partitioned $E\begin{Bmatrix}\psi\\ \Phi\end{Bmatrix} = \left[\begin{array}{c|c} H & \tau \\ \hline \tau^+ & H_1 + i0^+ \end{array}\right]\begin{Bmatrix}\psi\\ \Phi\end{Bmatrix}$
- Contact before being connected to channel: $(EI - H_1 + i0^+)\Phi_1 = 0$
- What happens after connection?

Schrödinger Equation

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- Schrödinger Equation becomes:

$$E\begin{Bmatrix}\psi\\ \Phi_1+\chi\end{Bmatrix}=\begin{bmatrix}H & \tau_1\\ \tau_1^+ & H_1-i0^+\end{bmatrix}\begin{Bmatrix}\psi\\ \Phi_1+\chi\end{Bmatrix}$$

- So we have:

$$E\psi=[H]\psi+[\tau_1]\chi+[\tau]\Phi_1$$

$$E\Phi_1+E\chi=[\tau_1^+]\psi+[H_1-i0^+]\Phi_1+[H_1+i0^+]\chi$$

- Since Φ_1 is an eigenstate of the reservoir,

$$\cancel{E\Phi_1}+E\chi=[\tau_1^+]\psi+\cancel{[H_1-i0^+]\Phi_1}+[H_1+i0^+]\chi$$

- Grouping the similar terms,

$$[E-H_1+i0^+]\chi=[\tau_1^+]\psi$$

- The solution is:

$$\chi=[G_1][\tau_1^+]\psi$$

- Substituting back into the first equation,

$$[EI-H-\Sigma_1]\psi=[\tau_1]\Phi_1$$

$$([\Sigma_1]=\tau_1 G_1 \tau_1^+)$$

- We are used to dealing with the Schrödinger equation like

$$[EI-H]\psi=0$$

But here we have a driven system that we solve for:

$$[EI-H-\Sigma_1]\psi=[\tau_1]\Phi_1$$

Towards Electron Density

• In case of two contacts, we would have:

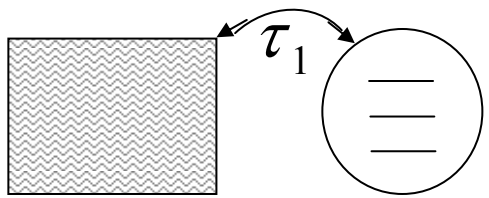
$$\left[EI - H - \Sigma_1 - \Sigma_2\right]\psi = \left[\tau_1\right]\Phi_1 + \left[\tau_2\right]\Phi_2$$

For now, we keep things simple and continue with one contact; solving for ψ, we have: $\psi = \left[G\right]S_1$

Where,

$\left(S_1 = \left[\tau_1\right]\Phi_1\right)$ and $G = \left(EI - H - \Sigma_1\right)^{-1}$

• Next step is to find the electron density inside the channel.



• There are millions of eigenstates inside the reservoir which we can denote by α and each of them has its own eigenvalue. i.e.

$$\left(E - \varepsilon_\alpha + i0^+\right)\Phi_\alpha = 0$$

and each solution will give rise to a certain ψ.

A Very Important Physical Concept

• We know that the net electron density is $\psi^*\psi$. Now the question is:

$\left|\sum_\alpha \psi_\alpha\right|^2$ or $\sum_\alpha \left|\psi_\alpha\right|^2$

Wrong Correct

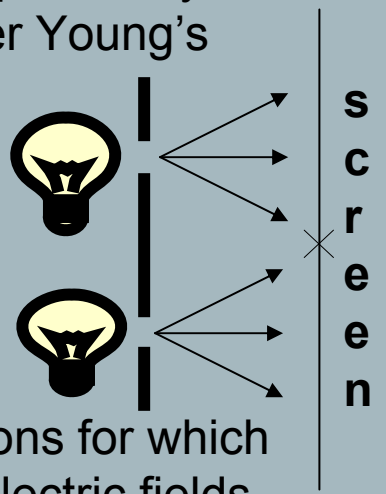
• Note that this is only true as long as α represents an eigenstate of the contact.

• The reason relies on coherence discussed on the next page.

Young's Double-Slit Experiment
Intensity vs. Electric Field

29:50

• There are lots of eigenstates in the contact, however there is NO coherence between them and in that sense they all act independently.
• For instance, consider Young's double-slit experiment:
• For thermal sources without coherence we should add intensities whereas for coherent sources like laser we might have had situations for which we'd want to add the electric fields.



• Electrons are more like thermal sources and they act incoherently.
• We should find ψ due to each excitation in the contact and then add the intensities (ψψ*).

$$\psi_\alpha = [G]S_\alpha$$

$$(S_1 = [\tau_1]\Phi_1)$$

$$\psi_\alpha = [G][\tau_1]\Phi_\alpha$$

• Electron Density

$$\{\psi_\alpha\}\{\psi_\alpha\}^+$$

$$\phi_2 \begin{Bmatrix} \times \\ \otimes \\ \times \\ \times \end{Bmatrix} \underset{\phi_3}{\{\times\times\otimes\times\}^*} \quad \text{Row } 2 \quad \text{Column } 3 \quad \phi_2\phi_3$$

=

• The significant ones from the point of view of electron density are the diagonal ones.

Total Number of Electrons

$$\{\psi_\alpha\}^+\{\psi_\alpha\} = Trace\left[\{\psi_\alpha\}\{\psi_\alpha\}^+\right]$$

Towards Density Matrix

- Based on $\psi_\alpha = [G][\tau_1]\Phi_\alpha$, we have:

$$\{\psi_\alpha\}\{\psi_\alpha\}^+ = [G][\tau_1]\Phi_\alpha\Phi_\alpha^+[\tau]^+[G]^+$$

- Summing over all states that are occupied,

$$\sum_\alpha f_1(\varepsilon_\alpha)\{\psi_\alpha\}\{\psi_\alpha\}^+ = \sum_\alpha f_1(\varepsilon_\alpha)[G][\tau_1]\Phi_\alpha\Phi_\alpha^+[\tau]^+[G]^+$$

Making use of the definition of delta function:

$$\left(\sum_\alpha f_1(\varepsilon_\alpha) = \int dE f_1(E)\sum_\alpha \delta(E-\varepsilon_\alpha)\right)$$

- We have:

$$\sum_\alpha f_1(\varepsilon_\alpha)\{\psi_\alpha\}\{\psi_\alpha\}^+ = \int dE f_1(E) G\tau_1 \underbrace{\sum_\alpha \Phi_\alpha\Phi_\alpha^+\delta(E-\varepsilon_\alpha)}_{\text{Spectral Function } [a_1]}\tau_1^+ G^+$$

Density Matrix

$$\sum_{\alpha} f_1(\varepsilon_\alpha)\{\psi_\alpha\}\{\psi_\alpha\}^+ = \int dE f_1(E) G \tau_1 \sum_{\alpha} \Phi_\alpha \Phi_\alpha^+ \delta(E-\varepsilon_\alpha)\tau_1^+ G^+$$

$$\Rightarrow \int dE G^n = \int dE f_1(E) G \underbrace{\tau_1 a_1 \tau_1^+}_{\Gamma_1} G^+$$

- We wanted to derive the electron density inside the channel:

$$G^n = ([A_1]f_1 + [A_2]f_2)$$
$$(G\Gamma_1 G^+ = A_1) \qquad (A_2 = G\Gamma_2 G^+)$$

- Note:

$$\Gamma_1 = i(\Sigma_1 - \Sigma_1^+) = i\left(\tau_1 G_1 \tau_1^+ - \tau_1 G_1^+ \tau_1^+\right) = \tau_1 a_1 \tau_1^+$$

$$\Sigma_1 = \tau_1 G_1 \tau_1^+ \quad \tau_1 G_1 \tau_1^+ = \Sigma_1^+$$

General Philosophy; Pauli Blocking?

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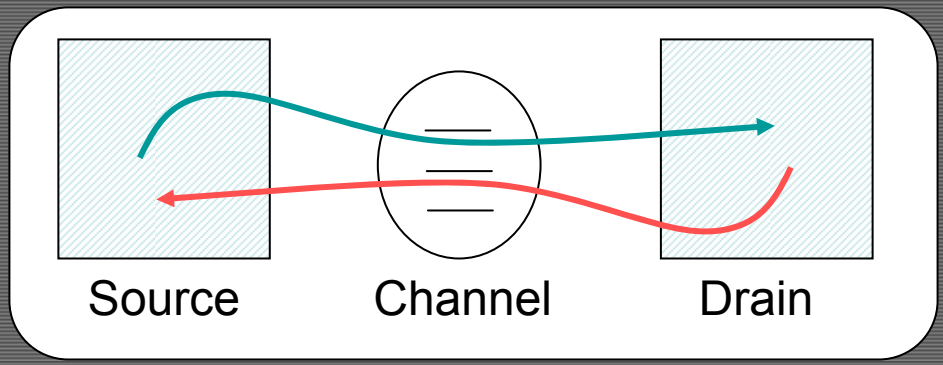

General Philosophy

- Start from something that describes the device and contact together.
- Contact is full of eigenstates which are trying to fill up the device; find the resulting wave function.
- Each eigenstate acts on the device independently.
- Do the states crossing from right to left and from left to right block one another because of Exclusion Principle?
- No. As long as you start from two states that are orthogonal, even if they overlap, they can't block each other.