Quantum Transport:
Atom to Transistor

Prof. Supriyo Datta
ECE 659
Purdue University

04.12.2004

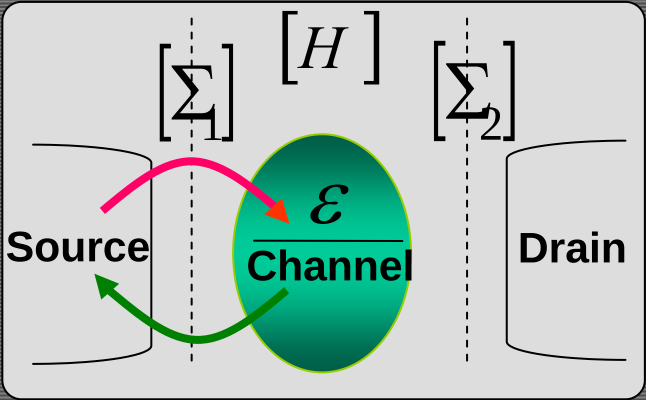
Lecture 33: Inflow / Outflow
Ref. Chapter 9.3

Network for Computational Nanotechnology

NCN nanoHUB online simulations and more

Matrix Version of Current

00:00



$$N = \int dE\, n(E)$$

$$n(E) = D(E)\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$$

$$I_j(E) = \int dE\, \tilde{I}_j(E)$$

$$\tilde{I}_j(E) = \underbrace{\gamma_j D f_j}_{IN} - \underbrace{\gamma_j n}_{OUT}$$

- Last day we derived the matrix version of n(E). Today we want to derive the matrix version of $\tilde{I}_j(E)$.
- For the matrix version, we have the Hamiltonian matrix which describes the channel and the two self energy functions which describe the coupling to the contacts.
- The broadening function Γ is related to the imaginary part of the self energy as $\Gamma_j = i\left(\Sigma_j - \Sigma_j^+\right)$
- We've written the matrix version of n(E) as

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

- The current's matrix equation:

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

- Where

$$G = \left(EI - H - \Sigma_1 + \Sigma_2\right)^{-1};\ A = i\left(G - G^+\right)$$

- In going through the derivation of matrix versions, we'll just think of ONE contact to make the algebra simpler.

Schrödinger Equation

06:00

- The Schrödinger equation for the system of channel and one contact is:

$$E\begin{Bmatrix}\psi \\ \Phi\end{Bmatrix} = \left[\begin{array}{c|c} H & \tau \\ \hline \tau^{+} & H_R \end{array}\right]\begin{Bmatrix}\psi \\ \Phi\end{Bmatrix}$$

- The approach is to think of the system in two steps before connection and after connection. With this strategy the wave function in the contact can be described by the summation of what it was before coupling and what was induced after connection.

$$\Phi = \Phi_R + \chi$$

- We'll have:

$$E\begin{Bmatrix}\psi \\ \Phi_R + \chi\end{Bmatrix} = \begin{bmatrix} H & \tau \\ \tau^{+} & H_R - i\eta \end{bmatrix}\begin{Bmatrix}\psi \\ \Phi_R + \chi\end{Bmatrix}$$

- Focusing on the channel's equation in this system of two equations, we have:

$$E\psi = (H + \Sigma)\psi + S$$

Where $\Sigma = \tau g_R \tau^{+}$

$$g_R = (EI - H_R + i\eta)^{-1}$$

$$S = \tau\Phi_R$$

- The device will react back on the contact and result in the induced term:

$$\chi = g_R \tau^{+} \psi$$

Density Matrix

14:10

- Next we want to derive the Density Matrix. As we know the density is defined as ψψ.* Density Matrix is a matrix whose (i, j)th component is $\rho_{ij} = \psi_i \psi_j^*$.

$$[\rho]: \quad \mathbf{i}\begin{pmatrix} & \overset{\mathbf{j}}{\otimes} & \\ & & \\ & & \end{pmatrix}$$

- Therefore density matrix can be written as: $[\rho] = \{\psi\}\{\psi\}^+ ; \rho_{ij} = \psi_i \psi_j^*$

- But could we write the density matrix like this? $[\rho] \overset{?}{=} \{\psi\}\{\psi\}^+$ This is not true.

- This just gives us a number (Trace of density matrix) NOT the density matrix itself.

- We can derive ψ from Schrödinger equation:

$$E\psi = (H + \Sigma)\psi + S \Rightarrow$$

$$(EI - H - \Sigma)\psi = S \Rightarrow$$

$$\psi = \underbrace{(EI - H - \Sigma)^{-1}} S = \underbrace{[G]}\{S\}$$

- For Density Matrix we then have:

$$[\rho] = GSS^+G^+ = G\tau\Phi_R\Phi_R^+\tau^+G^+;$$

Where,

$$(S = \tau\Phi_R) \quad (AB)^+ = B^+A^+$$

Two Points

19:00

Notation ① **Two Important Points** ② **Concept**

• What is $\{\psi\}_\alpha$?
Answer: It is a **column vector** describing the wave function inside the channel due to excitation by the (α)th eigenstate in the contact.

• What is ψ_α?
Answer: It is a **number.** It is the (α)th component of the wave function ψ inside the device.

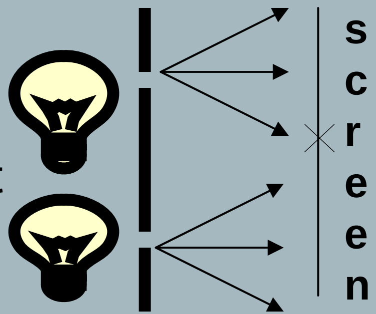
• Remember

$$\{\psi\}_\alpha \neq \psi_\alpha$$

• 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 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 (squares of the wave function).

Density Matrix

- So to get the total density matrix inside the channel we should add ψ ψ* and sum over all eigenvalues α corresponding to the occupied eigensates inside the contact.

$$[\rho] = \sum_{\alpha} f_0(\varepsilon_\alpha - \mu)\{\psi\}_\alpha \{\psi\}_\alpha^{+} = \sum_{\alpha} f_0(\varepsilon_\alpha - \mu) G S_\alpha S_\alpha^{+} G^{+}$$

$$[\rho] = \sum_{\alpha} f_0(\varepsilon_\alpha - \mu) G \tau \Phi_\alpha \Phi_\alpha^{+} \tau^{+} G^{+}$$

Converting to Integral

$$[\rho] = \int \frac{dE}{2\pi} f_0(\varepsilon_\alpha - \mu) \sum_{\alpha} G \underbrace{\tau \Phi_\alpha \Phi_\alpha^{+} \delta(E - \varepsilon_\alpha)}_{a_R} \tau^{+} G^{+}$$

a_R Tells us the DOS in the Reservoir

Since,

$$\Gamma = i\left(\Sigma - \Sigma^{+}\right) = i(\tau g_R \tau^{+} - \tau g_R^{+} \tau^{+}) = \tau i \overbrace{(g_R - g_R^{+})}^{a_R} \tau^{+} = \tau a_R \tau^{+}$$

We get: $$[\rho] = \int \frac{dE}{2\pi} f_0(\varepsilon_\alpha - \mu) \sum_{\alpha} G \Gamma G^{+};$$

Which is what we had before

$$G_1^n(E) = \left(G \Gamma_1 G^{+}\right) f_1$$

Definition of Current

28:00

- What we want to do today is to derive the current matrix equation; similar to the derivation of density matrix. In other words we want to derive:

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

  - **Question: What is the definition of the current? How do we define current?**

- In order to get the answer, we have to look at the time-dependent version of Schrödinger Equation:

$$i\hbar \frac{\partial}{\partial t}\begin{Bmatrix}\psi \\ \Phi\end{Bmatrix} = \begin{bmatrix} H & \tau \\ \tau^+ & H_R - i\eta \end{bmatrix}\begin{Bmatrix}\psi \\ \Phi\end{Bmatrix}$$

- Then we can ask the question: what is the rate at which the probability is changing inside the device. So this is what we want:

$$\frac{d}{dt}\left(\psi^+\psi\right)$$

- Note that ψ*ψ is a number.

$$\psi^+\psi = \sum_i \psi_i^* \psi_i$$

- **If the probability inside the device is changing, then there must be a current flow and calculating the rate at which this probability changes is a good measure of current.**

- On the next page we will derive an expression for $\frac{d}{dt}\left(\psi^+\psi\right)$ in terms of Hamiltonians and τ's.

Probability Current

Want to Find

$$\frac{d}{dt}\left(\psi^{+}\psi\right)$$

Chain Rule

$$\frac{d}{dt}\left(\psi^{+}\psi\right)=\frac{d\psi^{+}}{dt}\psi+\psi^{+}\frac{d\psi}{dt}$$

Conjugate of Schrödinger Equation

$$-i\hbar\frac{d}{dt}\psi^{+}=\psi^{+}H+\Phi^{+}\tau^{+}$$

$\times\Psi$

1

$$\psi^{+}H\psi+\Phi^{+}\tau^{+}\psi=-i\hbar\frac{d\psi^{+}}{dt}\psi$$

Schrödinger Equation

$$i\hbar\frac{d}{dt}\psi=H\psi+\tau\Phi$$

$\Psi^{*}\times$

2

$$\psi^{+}i\hbar\frac{d\psi}{dt}=\psi^{+}H\psi+\psi^{+}\tau\Phi$$

2 − 1 $\Longrightarrow$

$$\frac{d}{dt}\left(\psi\psi^{+}\right)=\frac{\psi^{+}\tau\Phi-\Phi^{+}\tau^{+}\psi}{i\hbar}$$

Current Matrix

33:15

- For current we then have:

$$I = Trace\left(\frac{\psi^{+}\tau\Phi - \Phi^{+}\tau^{+}\psi}{i\hbar}\right) \qquad \textbf{(1)}$$

- What we want to get at is like:

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

- To get the Inflow and Outflow, we'll replace Φ by $\Phi_R + \chi$ in **1**. The term that has Φ_R in it will be the Inflow and the one which has χ , will become Outflow.

$$\tilde{I}_j(E) = \underbrace{\overbrace{Trace\left[\Gamma_j A\right] f_j}^{\Phi_R}}_{\text{Inflow}} - \underbrace{\overbrace{Trace\left[\Gamma_j G^n\right]}^{\chi}}_{\text{Outflow}}$$

- Inflow and Outflow are calculated on the following pages.

Inflow

- **Expression For** I_{in}

$$\psi = GS \; ; \tau\Phi_R = S$$

$$I_{in} = Trace\left[\frac{\psi^+\tau\Phi_R - \Phi_R^{\;+}\tau^+\psi}{i\hbar}\right] = Trace\left[\frac{S^+G^+S - S^+GS}{i\hbar}\right]$$

$$= Trace\left[\frac{G^+SS^+ - GSS^+}{i\hbar}\right] = \sum_\alpha Trace\left[\frac{G^+S_\alpha S_\alpha^+ - GS_\alpha S_\alpha^+}{i\hbar}\right]$$

$$= \sum_\alpha f_0(\varepsilon_\alpha - \mu) Trace\left(\frac{G^+S_\alpha S_\alpha^+ - GS_\alpha S_\alpha^+}{i\hbar}\right)$$

$$S_\alpha S_\alpha^+ \rightarrow \Gamma f; \qquad \frac{G^+ - G}{i} \rightarrow A$$

$$= \frac{1}{\hbar}\int \frac{dE}{2\pi} f_0(\varepsilon_\alpha - \mu) Trace \sum_\alpha \frac{G^+ - G}{i} S_\alpha S_\alpha^+ \delta(E - \varepsilon_\alpha)$$

$$\frac{G^+ - G}{i} \longrightarrow A \qquad S_\alpha S_\alpha^+ \delta(E - \varepsilon_\alpha) \longrightarrow \Gamma$$

Inflow $\therefore \; I_{1in}(E) = \int dE \tilde{I}_{1in}(E) = \frac{1}{\hbar}\int \frac{dE}{2\pi} Trace\left[\Gamma_1 A\right] f_1$

Outflow

43:10

- **Expression For** I_{out}

$$\chi = g_R \tau^+ \psi$$

$$I_{out} = Trace\left[\frac{\psi^+ \tau\chi - \chi^+ \tau^+ \psi}{i\hbar}\right] = Trace\left[\frac{\psi^+ \tau g_R \tau^+ \psi - \psi^+ \tau g_\alpha^+ \tau^+ \psi}{i\hbar}\right]$$

$$= Trace\left[\frac{\tau g_R \tau^+ \psi\psi^+ - \tau g_R^+ \tau^+ \psi\psi^+}{i\hbar}\right] = \sum_\alpha Trace\left(\frac{\overbrace{\tau g_R \tau^+}^{\Sigma} \psi_\alpha \psi_\alpha^+ - \overbrace{\tau g_R^+ \tau^+}^{\Sigma^+} \psi_\alpha \psi_\alpha^+}{i\hbar}\right)$$

$$\Gamma = i\left(\Sigma - \Sigma^+\right), \sum_\alpha \psi_\alpha \psi_\alpha^+ = \int \frac{dE}{2\pi} G^n(E)$$

Outflow $\therefore I_{1out} = \dfrac{1}{\hbar}\displaystyle\int \frac{dE}{2\pi} \tilde{I}_{1out}(E) = \frac{1}{\hbar}\int \frac{dE}{2\pi} Trace\left(\Gamma G^n\right)$

Summary

47:50

How do we do the general problem of obtaining the matrix versions of our one level model equations?

- We've derived the expressions for electron density and current for the one-level device. We've then spent the rest of the course to figure out what Hamiltonian and self energy matrices are. Having these matrices, we have now derived the matrix versions of electron density inside the device and current through it. Well, how did we do this?
- We started with the Schrödinger equation for the whole system. We then partition the Schrödinger equation into two equations describing the channel and the contact. After that we eliminate the contact and focus on the channel with the idea that it started out empty and gets filled by the electron wave functions from the contact causing inflow. It then responded back and induces an electron wave function inside the contact causing outflow.
- To get the electron density or the current you DO NOT add up the wave functions, you add up the electron or current density i.e. you add up $\psi\psi^*$ instead of ψ's arising from each eigenstate of the contact.
- Once you've derived the equations, then you can use it for any device no matter how complicated it is.
- If H and Sigma could be diagonalized simultaneously, then we wouldn't need to go through all this to prove the matrix versions because we could write the equations for each diagonal element which would be INDEPENDENT and then you could just add them up. How ever this is NOT doable because in general H and Sigma cannot be diagonalized simultaneously.