Fundamentals of Nanoelectronics

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12.10.2004

Lecture 40: Summary
Ref.: Quantum Transport: Atom to Transistor
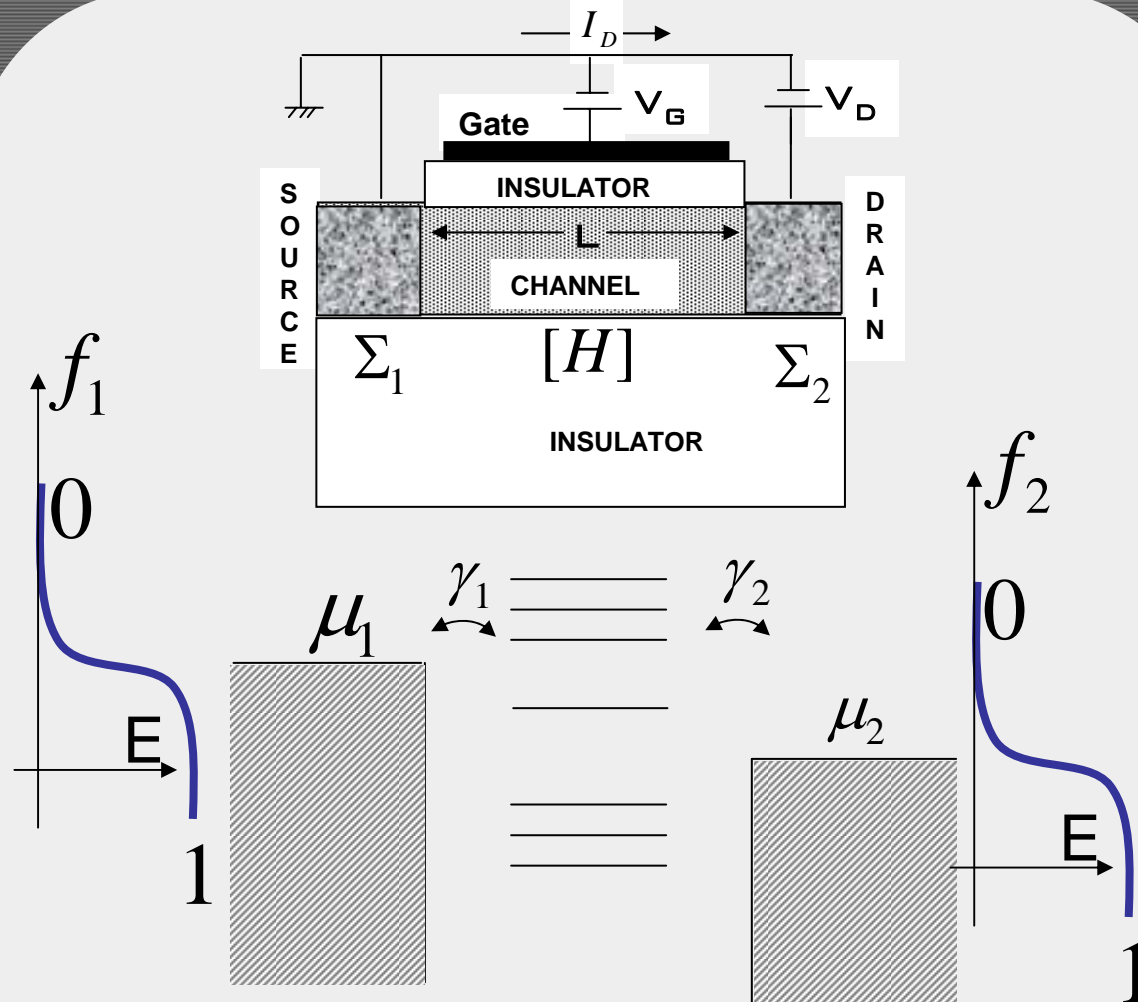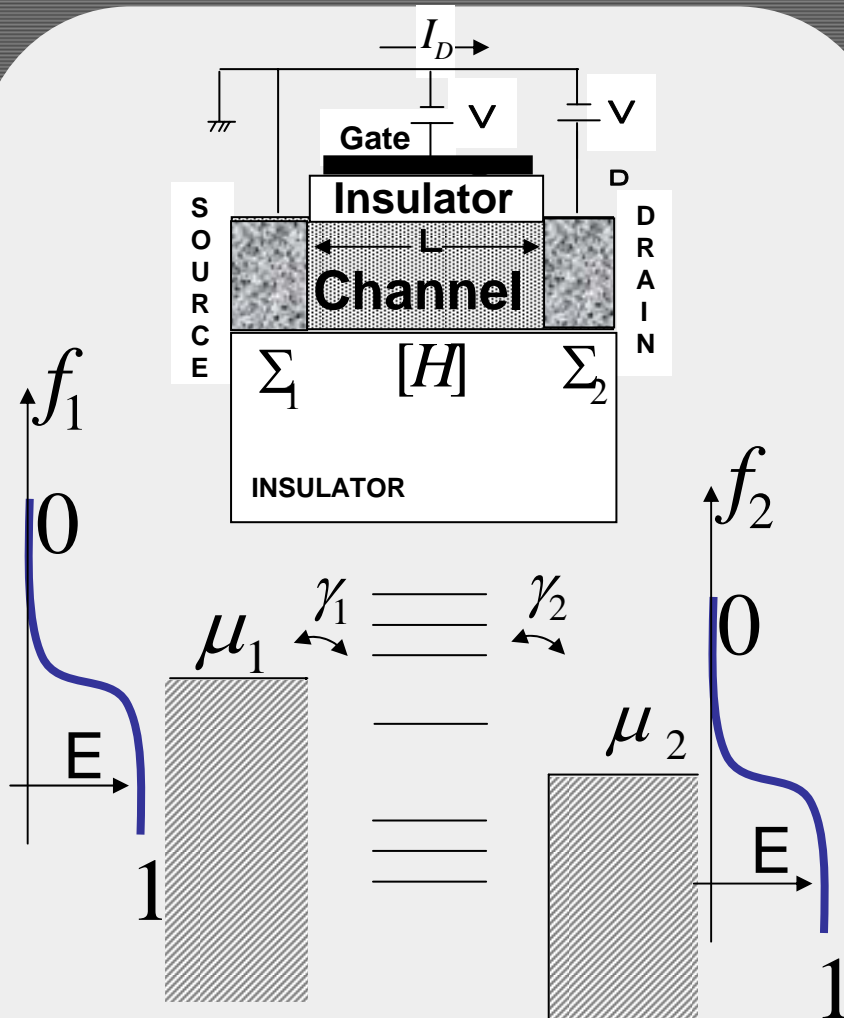
Network for Computational Nanotechnology

Model of a Nano Transistor
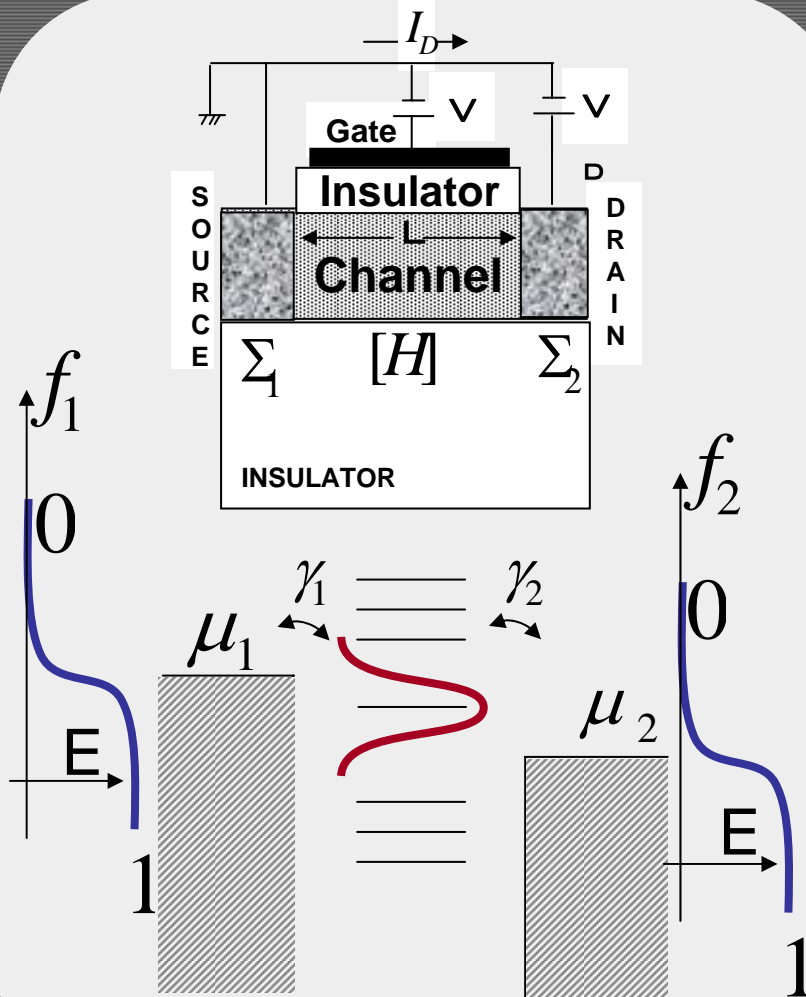
$$I_1 = q \frac{\gamma_1}{\hbar} (f_1 - N)$$

$$I_2 = q \frac{\gamma_2}{\hbar} (f_2 - N)$$

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

$$I = \frac{-q}{\hbar} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} (f_1 - f_2)$$
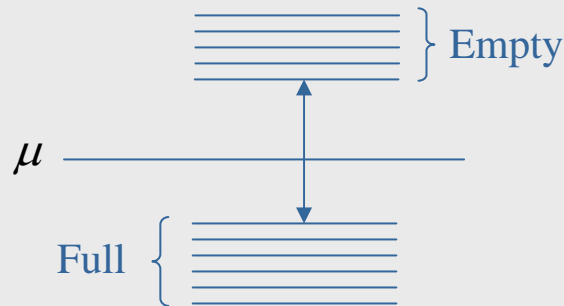
$$I_1 = q\,\frac{\gamma_1}{\hbar}(f_1 - N)$$

$$I_2 = q\,\frac{\gamma_2}{\hbar}(f_2 - N)$$

$$N = \int D(E)\,dE\,\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$$

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

μ

Empty

Full

• As we've been discussing, any material that forms the channel in a transistor can be visualized in terms of its energy levels. Current flow is introduction of an electron top one side of the channel and its going out from the other side. Any time an electron enters the channel, it has to go into an empty level. Talking out an electron involves and electron getting out of a filled level.

• Given a set of energy levels or Density of States (DOS), we've talked about the I-V characteristics of a device. What we want to understand now is how to model such energy levels / DOS.

• To achieve this, scientists started with the simplest material possible, namely the Hydrogen atom.
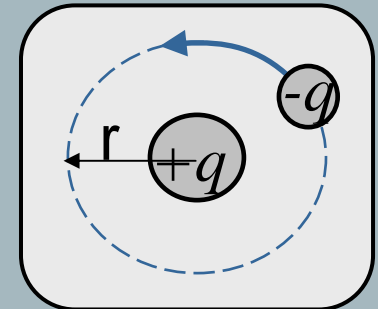
• A natural way to think about this atom is that the positive charge attracts the negative charge and the electron (negative charge) will circle around the proton kind of like rotation of earth around sun.

$$E_n = \frac{-Zq^2}{8\pi\varepsilon_0 r_n} = -\frac{Z^2}{n^2}\frac{q^2}{8\pi\varepsilon_0 a_0}$$

• What we had was:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}) \right]\psi = E\psi$$

• The basic idea for any method of numerical solution to the differential equation is to turn it into a matrix equation. We'll consider the finite difference method here. We'll end up with:

$$E\begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix} = \begin{bmatrix} \text{N by N} \end{bmatrix}\begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix}$$
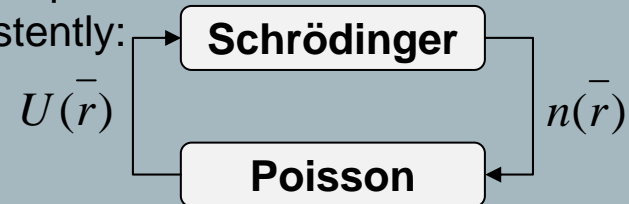
• Going from H atom to more complicated atoms, we have to consider the potential due to other electrons in addition to the nucleus potential…
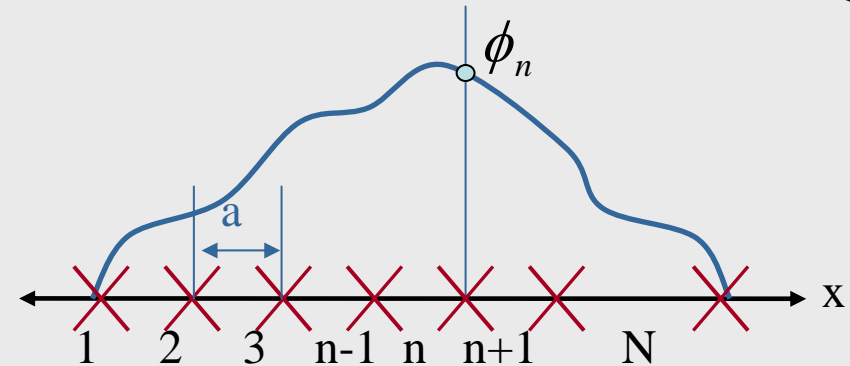
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U_N(\vec{r}) + U_{scf}(\vec{r}) \right]\psi = E\psi$$

• This equation has to be solved self consistently:

Schrödinger

$U(\bar{r})$

$n(\bar{r})$

Poisson

$$N = \int dE\, D(E)\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$$

$$U = U_L + U_0(N - N_0)$$

• Finite difference method gets out of hand for 3D solids. Calculating the eigenvalues of huge matrices resulting from FDM is hard if not impossible for computers.

• Thus we try to solve the problem in another way using the idea of basis functions.

• Schrödinger Equation: $H_{op} \phi_\alpha = E_\alpha \phi_\alpha$
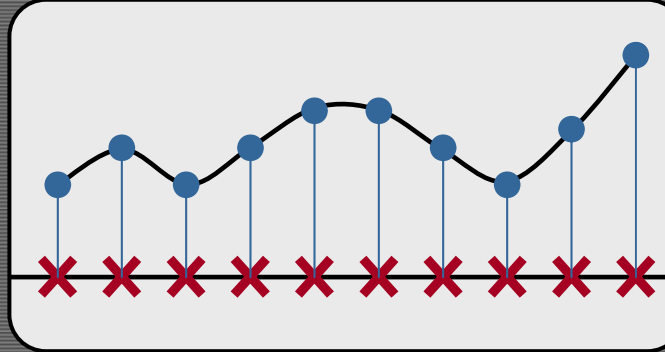
Whereby H_{op} is converted into a matrix and ϕ_α is a wavefunction represented spatially point by point

• Φ_α can be written as a linear combination of a set of basis functions:

$$\Phi_\alpha(\vec{r}) = \sum_m \phi_m u_m(\vec{r})$$

Where ϕ_m are coefficients and $u_m(\vec{r})$ are basis functions. So we can represent the wavefunction as a column vector with expansion coefficients as its elements:

$$\Phi(\vec{r}) \rightarrow \{\phi_1 \quad \phi_2 \quad ... \quad ... \quad \phi_M\}^T$$

• The principle of bandstructure helps us to find the eigenvalues of a periodic matrix. This is important for us because solids that we are interested in have periodic structures. Consider this example:

$$E \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix} = \begin{bmatrix} \varepsilon & t & 0 & 0 & 0 & 0 \\ t & \varepsilon & t & 0 & 0 & 0 \\ 0 & t & \varepsilon & t & & \\ 0 & & \ddots & \ddots & \ddots & \\ 0 & & & & & \\ 0 & & & & & \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix}$$

1s   1s   • • •   X

1   2   3   n-1   N
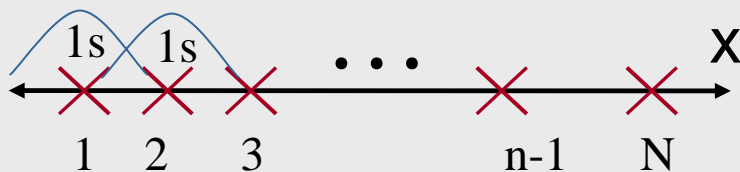
• Regardless of the details of the problem, the matrix that we write will be periodic.

• Notice that as long as every row looks the same, the principle of bandstructure applies regardless of how each row looks. The nth row is:

$$E\phi_n = t\phi_{n-1} + \varepsilon\phi_n + t\phi_{n+1} \quad (1)$$

• This solution satisfies the Schrödinger equation if the E-k relationship below is met.

$$\phi_n = e^{inka}\phi_0 \quad (2)$$

$$E = te^{-ika} + \varepsilon + te^{ika}$$

• 2 in 1 →

$$\boxed{E = \varepsilon + 2t\cos ka}$$

• As long as the above E-k relationship is met, the solution we chose will satisfy the Schrödinger equation.

• Often we are interested in low dimensional structures such as carbon nano-tubes. A low dimensional structure is that for which one or more dimension is very small.

• For the most part, if one or more dimension is on the nm scale (≈100 atoms) the conventional E-k diagram is not sufficient

• For confined structures we can categorize the eigen energies as follows:

$$\text{Bulk Solid}: E(k_x, k_y, k_z)$$
$$\text{Q. Well}: \quad E_v(k_x, k_y)$$
$$\text{Q. Wire}: \quad E_{v,v'}(k_x)$$
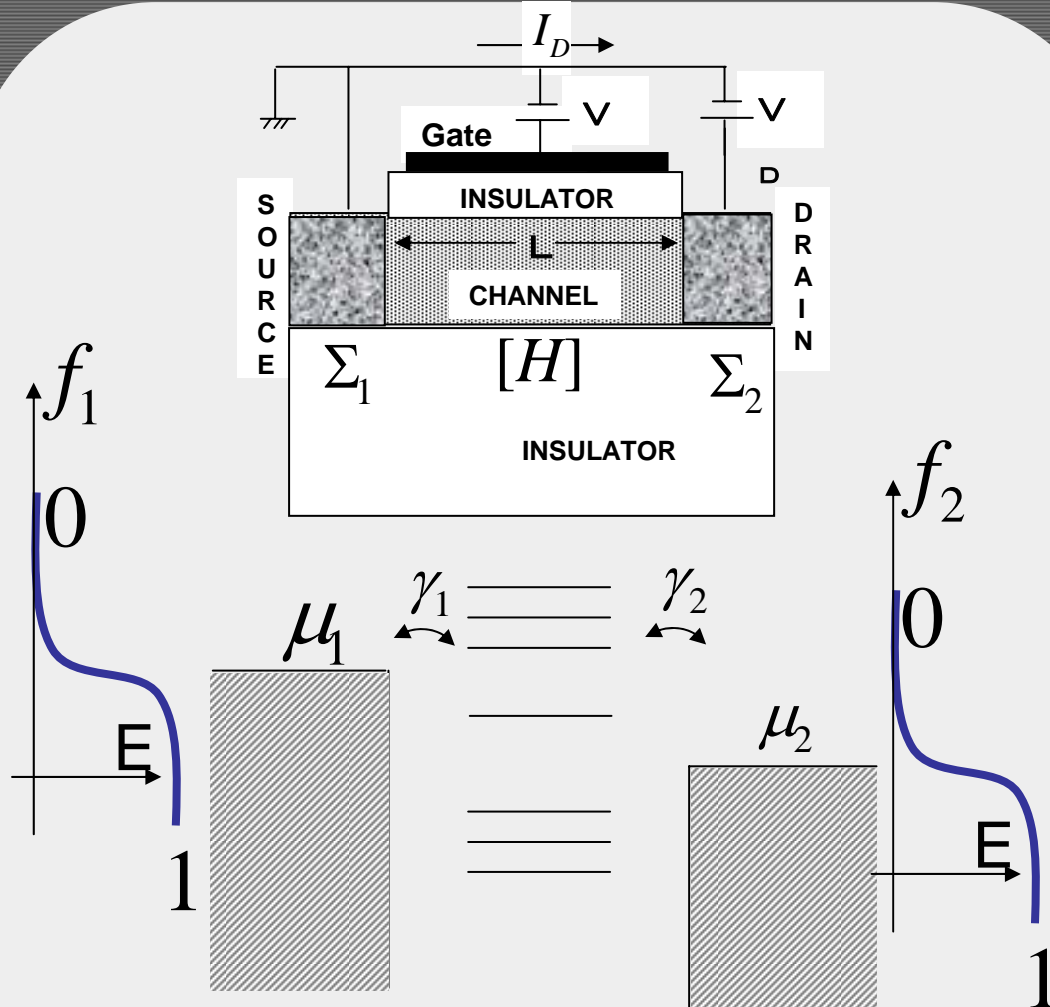$$\text{Q. Dot}: \quad E_{v,v',v''}$$

$$E_v(k_x, k_y) = E\left(k_x, k_y, k_z = \frac{v\pi}{L_z}\right)$$

$$E_{v,v'}(k_x) = E\left(k_x, k_y = \frac{v'\pi}{L_y}, k_z = \frac{v\pi}{L_z}\right)$$

$$E_{v,v',v''} = E\left(k_x = \frac{v''\pi}{L_x}, k_y = \frac{v'\pi}{L_y}, k_z = \frac{v\pi}{L_z}\right)$$

• Next we'd like to explain how Σ is related to lifetime.

• Let's start with Schrödinger equation: (suppose the channel is isolated form the contact)

$$i\hbar\frac{d\psi}{dt} = H\psi, \text{ Let } H = \varepsilon, \text{ then } \psi(t) \text{ can be written as } \psi(t) = \psi(0)e^{\frac{-i\varepsilon}{\hbar}t}$$

• Remember that we described the effect of the contact by the term Σ . If add this to H we get:

$$i\hbar\frac{d\psi}{dt} = H\psi; H = \varepsilon + \Sigma, \text{ then } \psi(t) = \psi(0)e^{\frac{-i\varepsilon}{\hbar}t}e^{\frac{-i\Sigma}{\hbar}t}$$

• If Σ is real, then there has been a shift in the energy and not much has changed. But if Σ has an imaginary part, then a DECAY factor is involved.

$$\left.\begin{array}{l} \psi(t) = \psi(0)e^{\frac{-i\varepsilon}{\hbar}t}e^{\frac{-i\Sigma}{\hbar}t} \\ \varepsilon' = \varepsilon + \text{Re }\Sigma \\ \gamma/2 = -\text{Im }\Sigma \end{array}\right\} \psi(t) = \psi(0)e^{\frac{-i\varepsilon'}{\hbar}t}e^{-\frac{\gamma}{2\hbar}t} \Rightarrow |\psi(t)|^2 = |\psi(0)|^2 e^{-\gamma t/\hbar}$$

• The electron density is the magnitude of psi^2 (see above). The expression for electron density shows the significance of the imaginary part of Σ . If there is not a coupling between the contact and channel the electron density remains constant. But if there is an imaginary part, the electron density has finite lifetime and it decays with time.

• We just learned that the imaginary part of Σ results in a finite lifetime. Another aspect of this is broadening. Early on in the course we discussed that if we connect the channel to a contact then, then the levels in the channel gets broadened. We stated that the a single sharp energy level looses a fraction of its value but then some fraction of energy levels from the contact spill over in the channel. As the result we had a broadening. The important point was that what the channel level looses at a particular energy, it gains the same amount at other energies so that the sum of the new distribution of energy levels adds up to 1 which is the value it had before connecting the channel to the contact.

• It is very important to keep broadening in the whole picture. Without it the value of calculated current will be wrong.
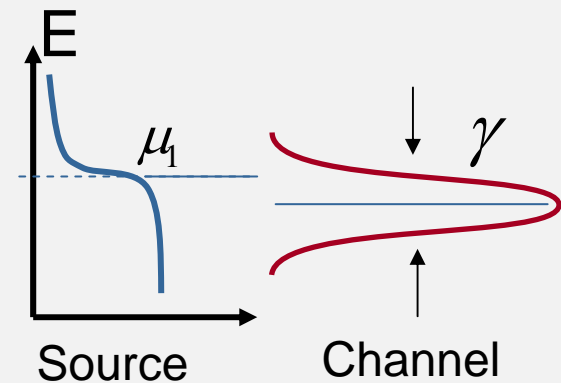
Source   Channel

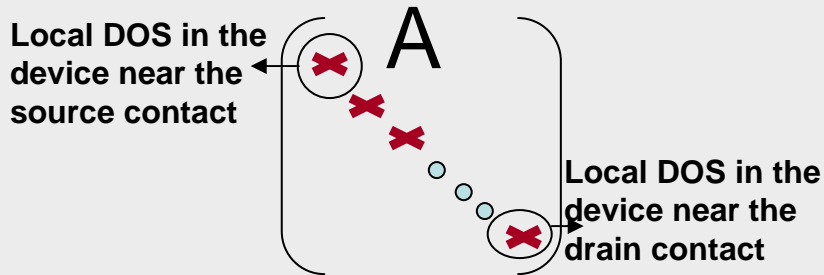$$G(E) = (EI - H - \Sigma_1 - \Sigma_2)^{-1}$$

$$A(E) = i(G - G^+)$$

$$\Gamma_1 = i(\Sigma_1 - \Sigma_1^+), \quad \Gamma_2 = i(\Sigma_2 - \Sigma_2^+)$$

$$[\rho] = \int \frac{dE}{2\pi} \left(\left[G\Gamma_1 G^+ \right] f_1 + \left[G\Gamma_2 G^+ \right] f_2 \right)$$

$$I = -\frac{q}{h} \int \frac{dE}{2\pi} Trace \left[\Gamma_1 G \Gamma_2 G^+ \right] (f_1 - f_2)$$

Local DOS in the device near the source contact

A

Local DOS in the device near the drain contact

• The general definition of DOS is:

$$D(E) = \sum_{\alpha} \delta(E - \varepsilon_{\alpha})$$

• What the above equation tells us is the average number of states over the entire solid. However for nanostructures we are interested in local density of states. Notice that even for large solids the density of states changes on atomic scale. This is important because current depends on density of states. In the figure below when the tip is on top of atoms, density of states is higher and there is more current flow.
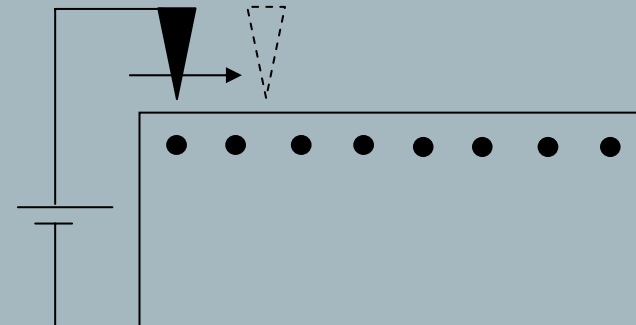
$$I_1 = q \frac{\gamma_1}{\hbar} (f_1 - N)$$

$$I_2 = q \frac{\gamma_2}{\hbar} (f_2 - N)$$

$$N = \int D(E) dE \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$$

$$I = \frac{-q}{\hbar} \int dE D(E) \underbrace{\frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2}}_{T(E)} (f_1 - f_2)$$

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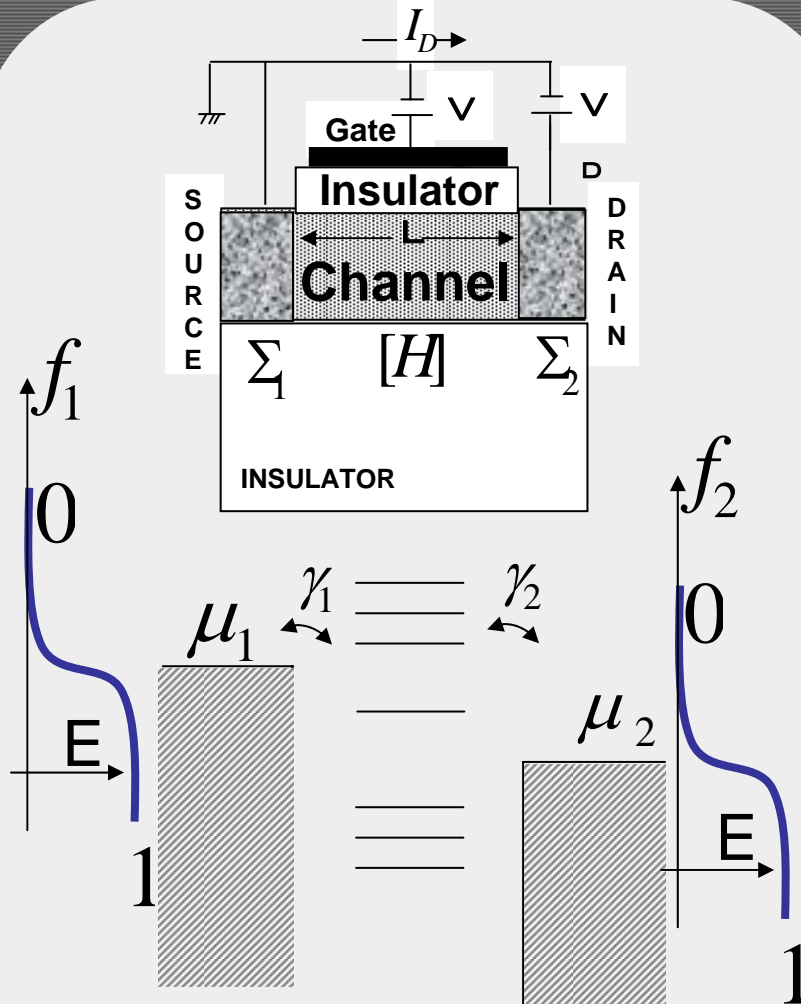
$$A(E) = i(G - G^+)$$

$$\Gamma_1 = i(\Sigma_1 - \Sigma_1^+)$$
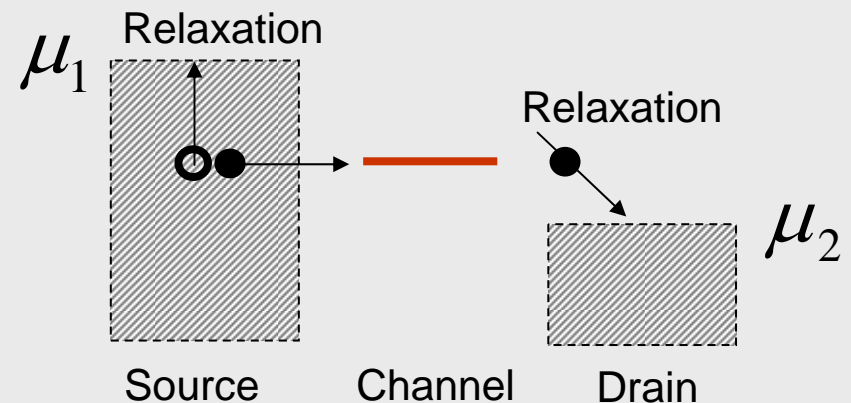
$$\Gamma_2 = i(\Sigma_2 - \Sigma_2^+)$$

$$[\rho] = \int \frac{dE}{2\pi} \left(\left[G\Gamma_1 G^+ \right] f_1 + \left[G\Gamma_2 G^+ \right] f_2 \right)$$

$$I = -\frac{q}{h} \int \frac{dE}{2\pi} \underbrace{Trace \left[\Gamma_1 G \Gamma_2 G^+ \right]}_{\overline{T}(E) = MT} (f_1 - f_2)$$
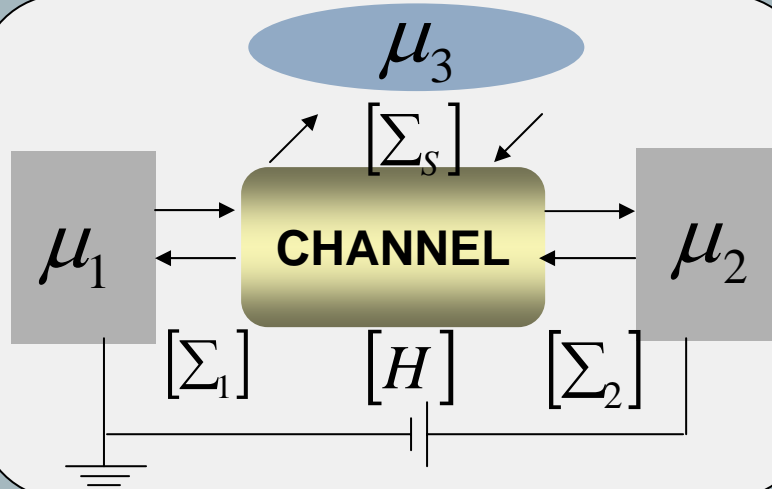
- *Basic Definition*: phonons are the lattice vibrations (sound) which propagate through a solid or molecule
- For example, hydrogen molecules vibrate about an equilibrium bond distance, R_{eq}, with an intensity proportional to temperature much like a spring mass system

$$\mu_3$$

$$[\Sigma_s]$$

CHANNEL

$$\mu_1 \qquad \mu_2$$

$$[\Sigma_1] \qquad [H] \qquad [\Sigma_2]$$

• Scattering processes can be taken into account in an indirect way by assuming a conceptual (not real) scattering contact. Electrons get in and get out of this contact with their phases randomized.

• Remember the old expression for current:

$$I = \frac{2q}{h} \int dE \, \overline{T}(E)\left(f_1(E) - f_2(E)\right)$$

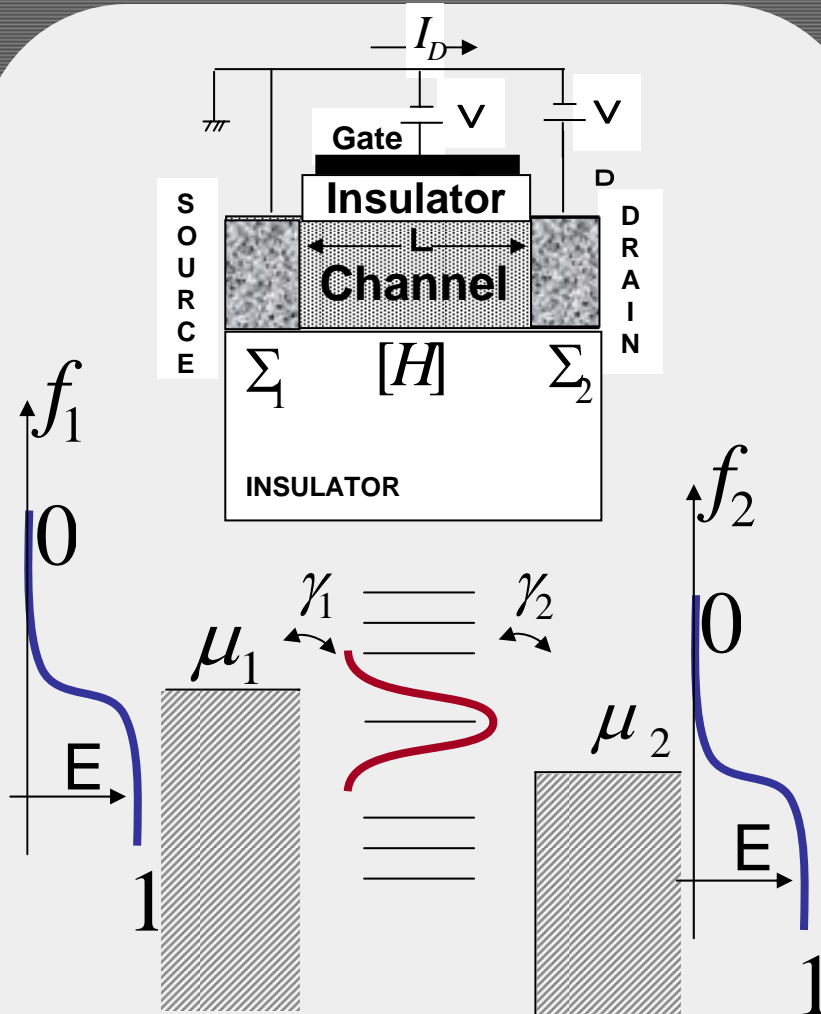• When the third contact is introduced the new equation for current at a terminal can be written as:

$$I_i = \frac{2q}{h} \int dE \sum_j \overline{T}_{ij}(E)\left(f_i - f_j\right)$$

• Notice that we do know the where the Fermi Levels $\mu 1$ and $\mu 2$ lie; however we don't know the position of $\mu 3$. The way we can find it is by knowing that the current going to the third contact is 0. So we adjust $\mu 3$ in way to get I3=0.

$$I_3 = \frac{2q}{h} \int dE \sum_j \overline{T}_{3j}(E)\left(f_3 - f_j\right) = 0$$

- The first thing we'd like to know is under what conditions coulomb blockade is important and has to be accounted for in modeling.
- Coulomb blockade becomes important when the coupling to the contacts and kT become much less than the single electron charging energy:

$$\gamma = \gamma_1 + \gamma_2$$

$$\gamma, k_B T << U_0$$

- Notice that the absence or presence of an electron in the channel results in raising or lowering of the level. The way we can account for this effect is:
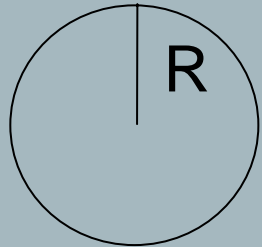
$$U = U_L + U_0 \Delta n$$

- U0 tells how much the potential changes if the number of electrons changes by 1.

- To get an order of magnitude estimation for U0, consider a sphere of charge.

$$U = \frac{q^2}{4\pi\varepsilon R}$$

$$U = \frac{1.6\times10^{-19}\,coul}{4\times3.14\times8.85\times10^{-12}\,\frac{F}{m}\times10^{-7}\,m}$$
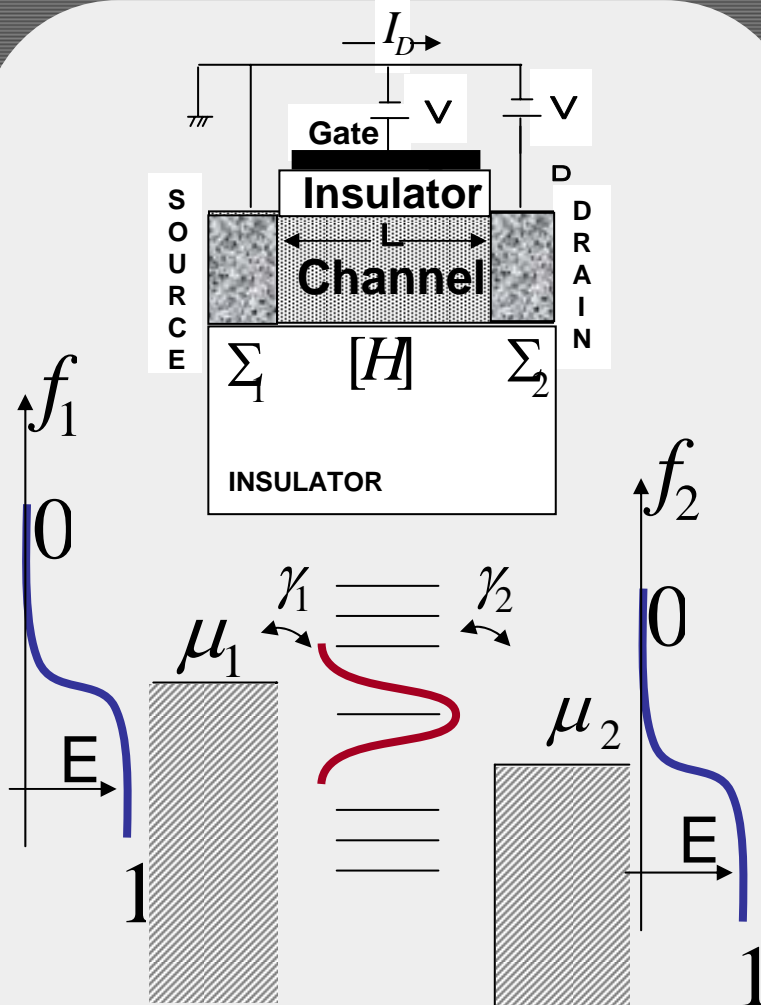
$$U \approx 14\,meV$$

- This is in the order of kT which is 25 meV at room temperature.
- R was taken to be 1000 Å. If larger, then U0 will even be smaller. This means that anytime an electron is added to the channel the amount of potential doesn't change much.
- We can see that for small devices, U0 will be larger and can affect the physical picture.

- Coulomb blockade becomes important if the following condition is **NOT** the case

$$\gamma, k_B T << U_0$$

$$G(E) = \left(EI - H - \sum\nolimits_1 - \sum\nolimits_2\right)^{-1}$$

$$A(E) = i(G - G^+)$$

$$\Gamma_1 = i(\Sigma_1 - \Sigma_1^+)$$

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

$$[\rho] = \int \frac{dE}{2\pi}\left(\left[G\Gamma_1 G^+\right]f_1 + \left[G\Gamma_2 G^+\right]f_2\right)$$

$$I = -\frac{q}{h}\int \frac{dE}{2\pi}Trace\left[\Gamma_1 G\Gamma_2 G^+\right](f_1 - f_2)$$