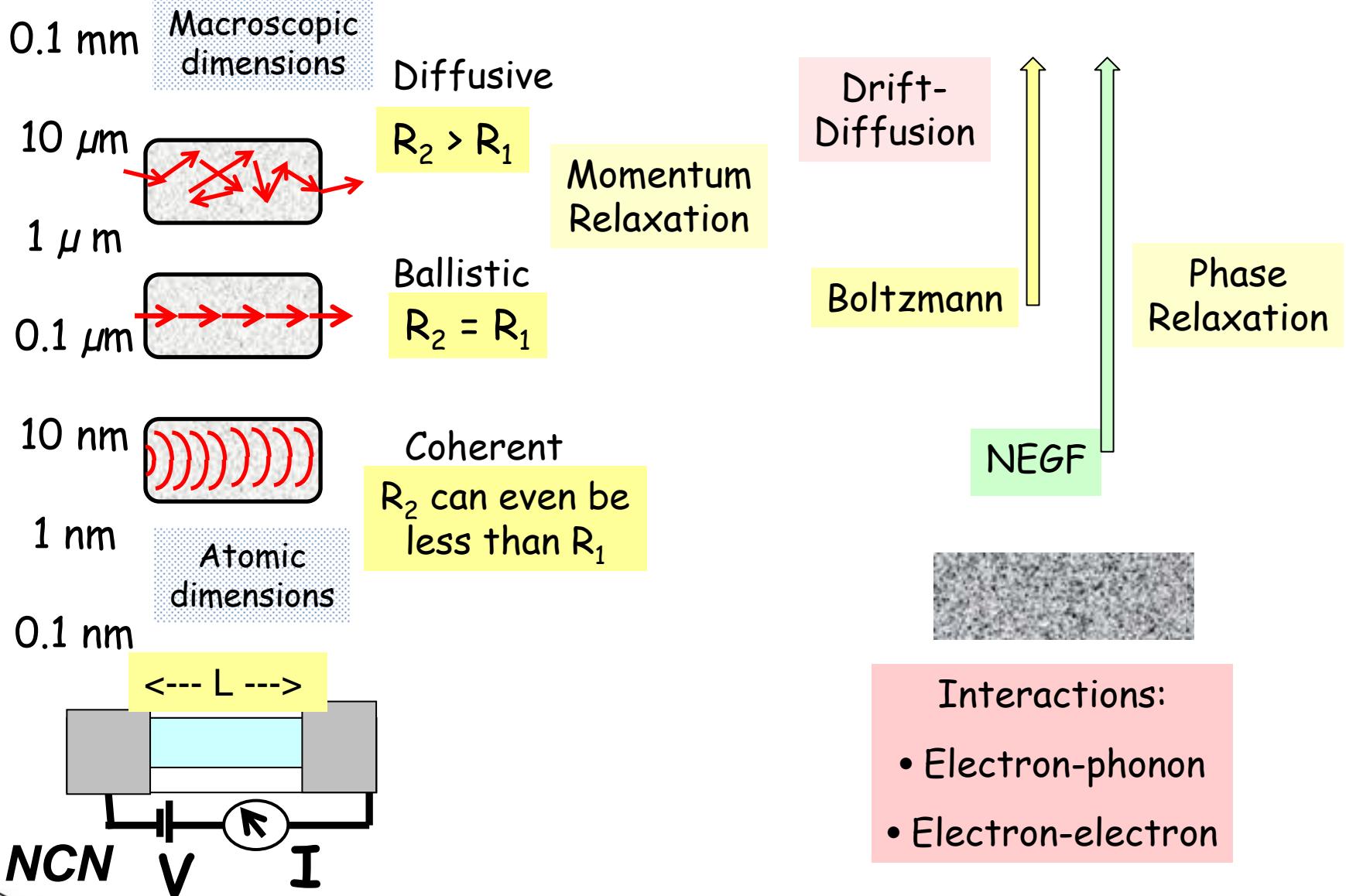
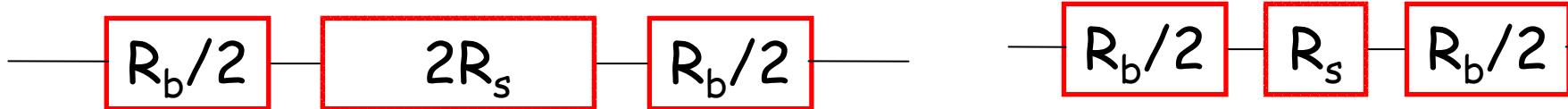


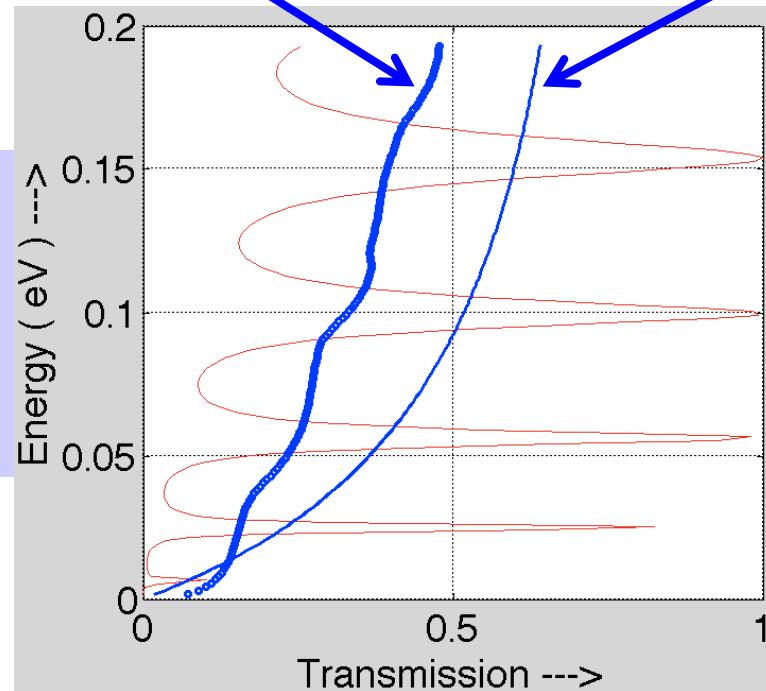
Bridges: Bottom to Top **



Towards Ohm's law



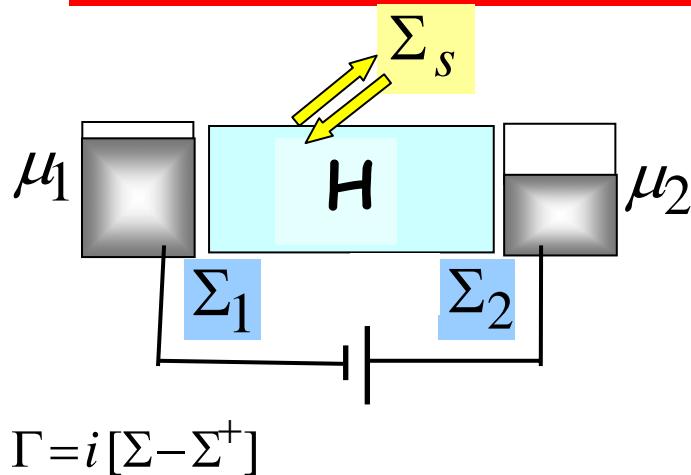
Phase relaxation
→Averages out
fluctuations



NCN



** NEGF equations with dephasing



$$\Gamma = i[\Sigma - \Sigma^+]$$

$$\varepsilon \rightarrow [H]$$

$$\gamma \rightarrow [\Gamma], [\Sigma]$$

$$n(E) \rightarrow [G^n(E)]$$

$$D(E) \rightarrow [A(E)]$$

Green
function

$$[G] = [EI - H - \Sigma_1 - \Sigma_2 - \Sigma_s]^{-1}$$

"Density of states" $A = i[G - G^+]$

"Electron density"

$$G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1 + G\Sigma_s^{in} G^+$$

Current

$$\frac{I_1}{q/\hbar} = \text{Trace} \left([\Gamma_1 A] f_1 - [\Gamma_1 G^n] \right)$$

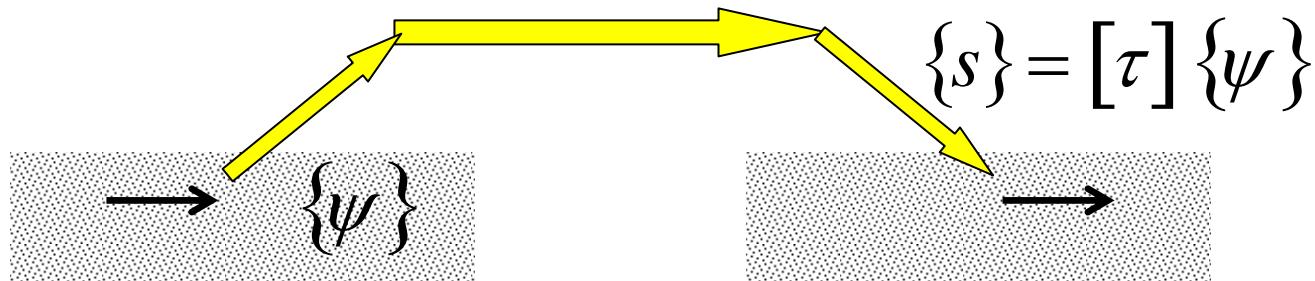
Dephasing model:

$$[\Sigma_s^{in}] = D [G^n]$$

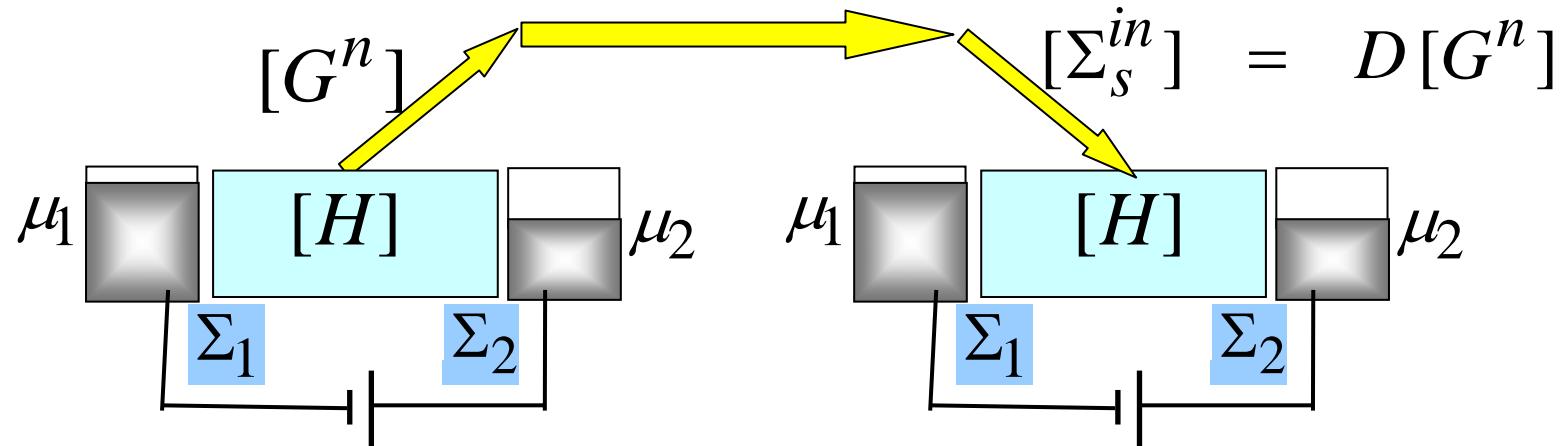
NCN



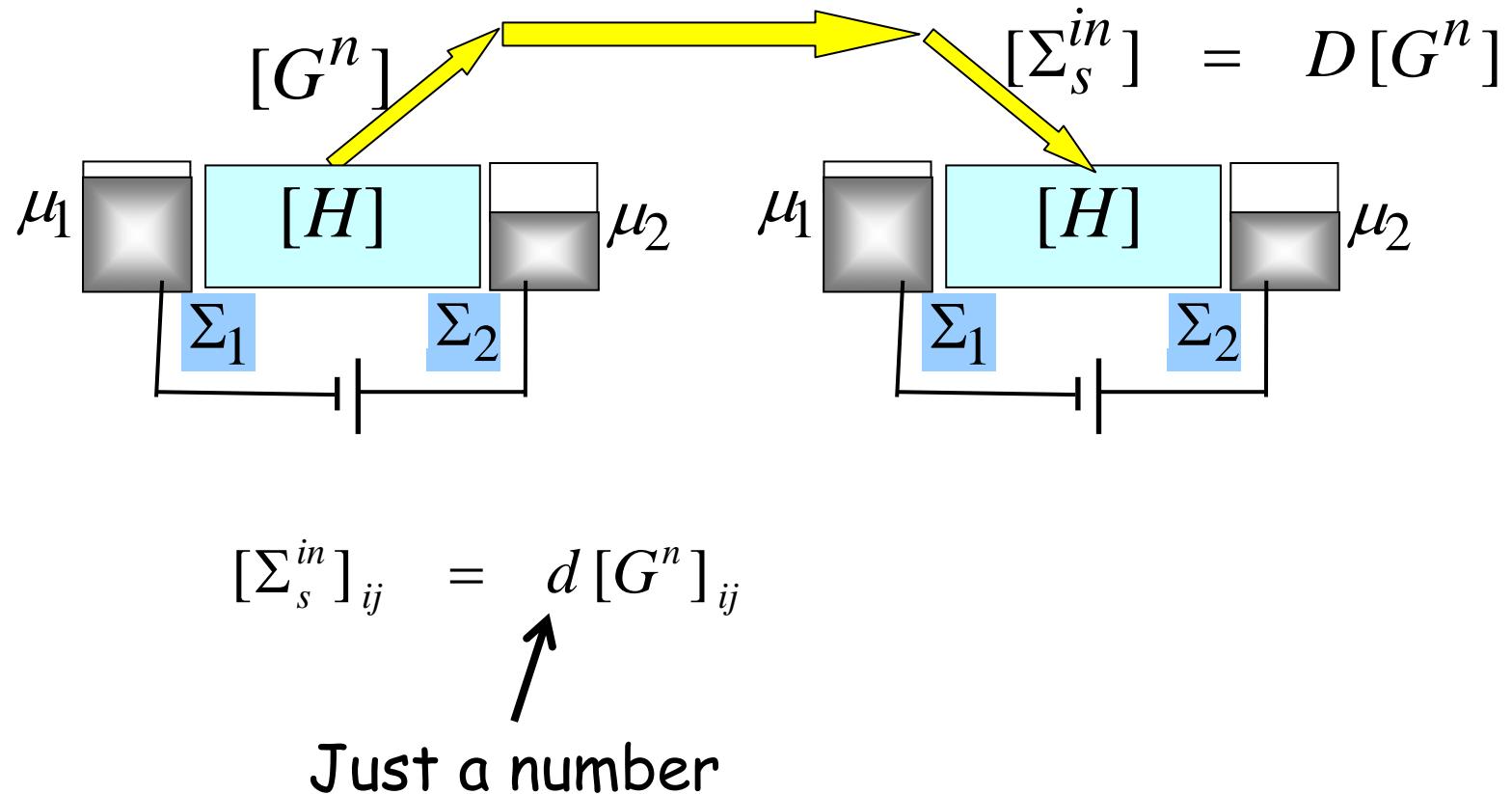
Dephasing: extraction and reinjection



$$\Sigma_s^{in} = \{s\}\{s\}^+ = [\tau] \begin{matrix} 1 & 4 \\ 4 & 2 \\ G^n \end{matrix} \begin{matrix} 1 & 4 \\ 2 & 3 \end{matrix}^+ [\tau]^+ \rightarrow \left[\Sigma_s^{in} \right]_{ij} = \begin{matrix} 1 & 4 \\ 4 & 2 \end{matrix}_{ik} \begin{matrix} \tau^+ \\ 4 & 3 \end{matrix}_{lj} \left[G^n \right]_{kl} D_{ijkl}$$



Pure phase relaxation



Off-diagonal elements carry momentum information

$\exp(+ikx) \rightarrow$



$\leftarrow \exp(-ikx)$

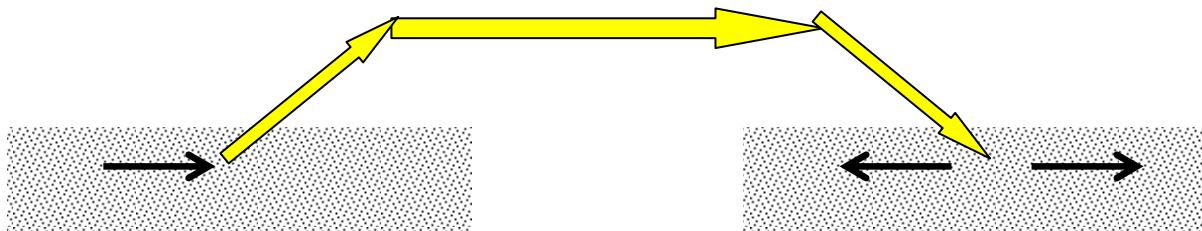
Correlation function

$$G^n = \{\psi\}\{\psi^+\} = \begin{bmatrix} \psi_1 \psi_1^* & \vdots & \psi_1 \psi_N^* \\ \vdots & \ddots & \vdots \\ \psi_N \psi_1^* & \vdots & \psi_N \psi_N^* \end{bmatrix}$$

$$[\Sigma_s^{in}]_{ij} = d [G^n]_{ij}$$

Just a number

Phase /Momentum relaxation



Momentum
Relaxation

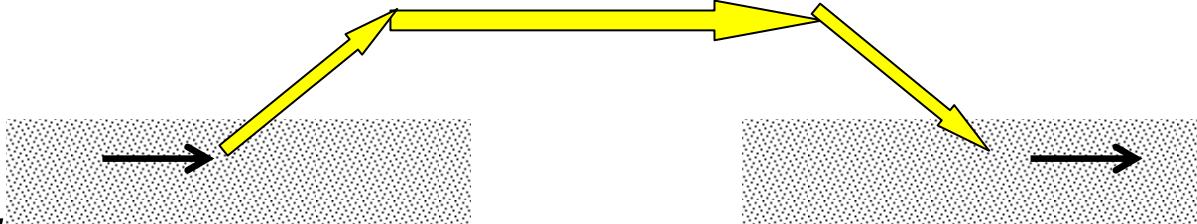
If only diagonal elements
are transferred

$$[\Sigma_s^{in}]_{ij} = d_m [G^n]_{ij} \delta_{ij}$$

Pure phase
Relaxation

If entire matrix is
transferred faithfully

$$[\Sigma_s^{in}]_{ij} = d [G^n]_{ij}$$

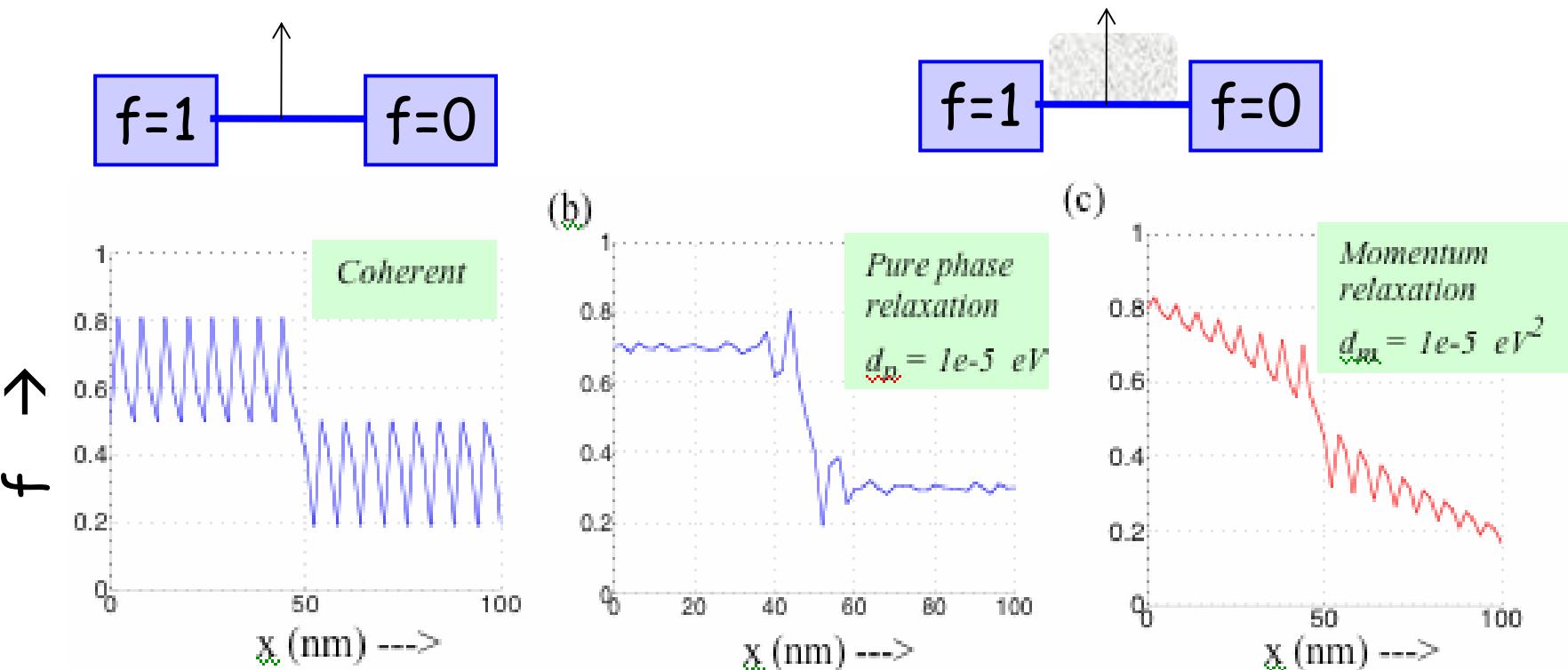


Golizadeh-Mojarad
and Datta,
Phys.Rev.B (2007)

NCN

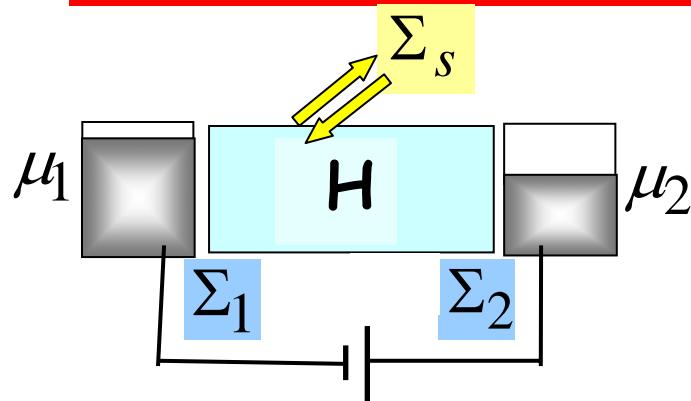


Potential drop across a scatterer



$$f(i) = \frac{n(i)}{D(i)} \rightarrow \frac{G^n(i,i)}{A(i,i)}$$

** NEGF equations with dephasing



$$\Gamma = i[\Sigma - \Sigma^+]$$

$$\varepsilon \rightarrow [H]$$

$$\gamma \rightarrow [\Gamma], [\Sigma]$$

$$n(E) \rightarrow [G^n(E)]$$

$$D(E) \rightarrow [A(E)]$$

Green
function

$$[G] = [EI - H - \Sigma_1 - \Sigma_2 - \Sigma_s]^{-1}$$

"Density of states" $A = i[G - G^+]$

"Electron density"

$$G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1 + G\Sigma_s^{in} G^+$$

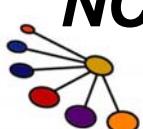
Current

$$\frac{I_1}{q/\hbar} = \text{Trace} \left([\Gamma_1 A] f_1 - [\Gamma_1 G^n] \right)$$

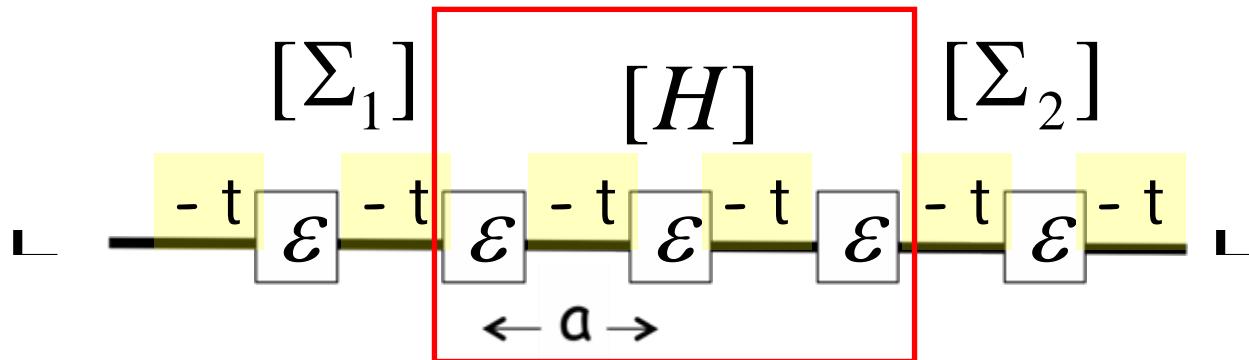
Dephasing model: $[\Sigma_s^{in}] = D [G^n]$

- Semi-empirical
- First principles

NCN



Tight-binding model (1-D)

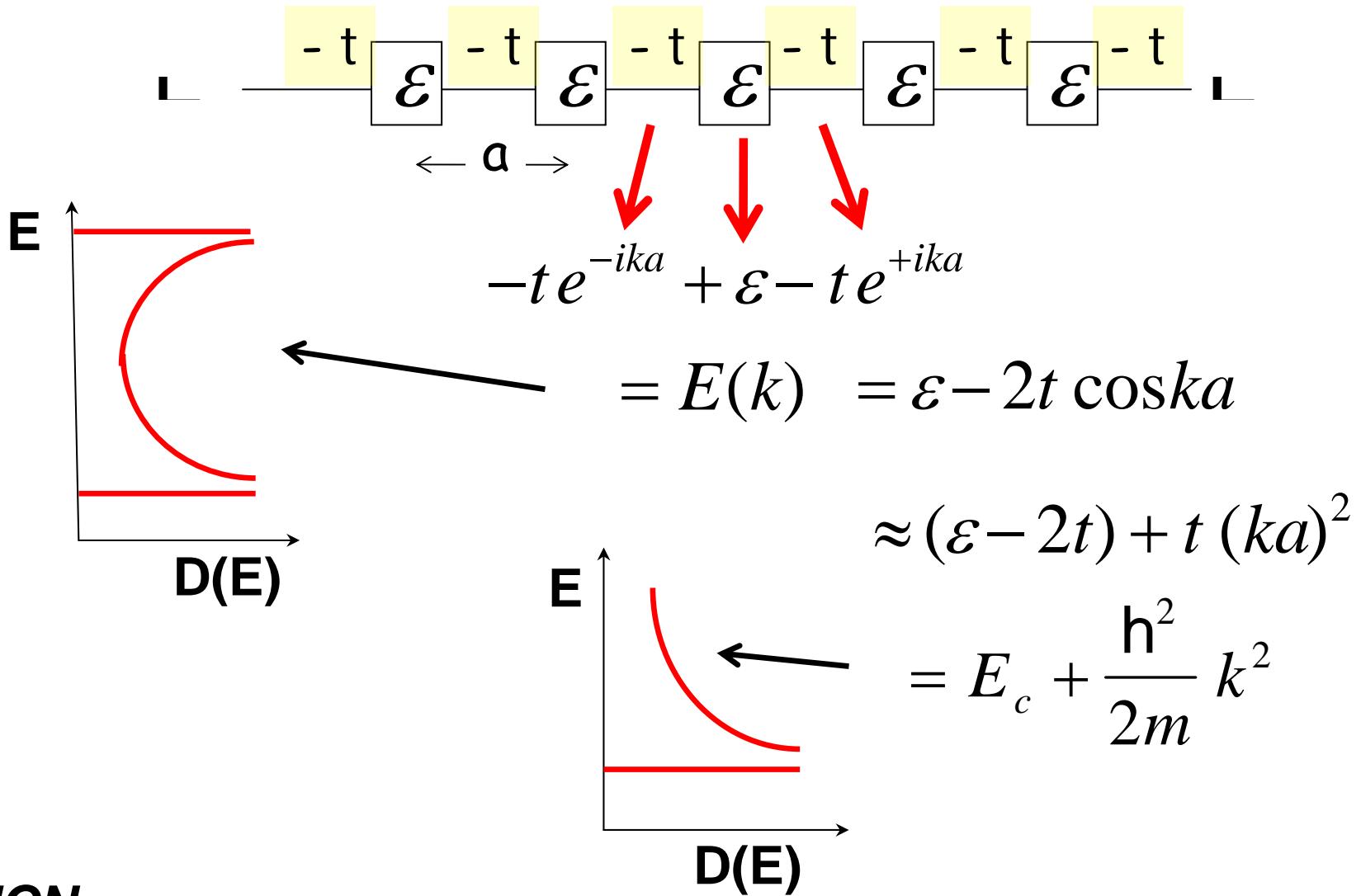


$$\Sigma_1(E) = \begin{bmatrix} ** & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

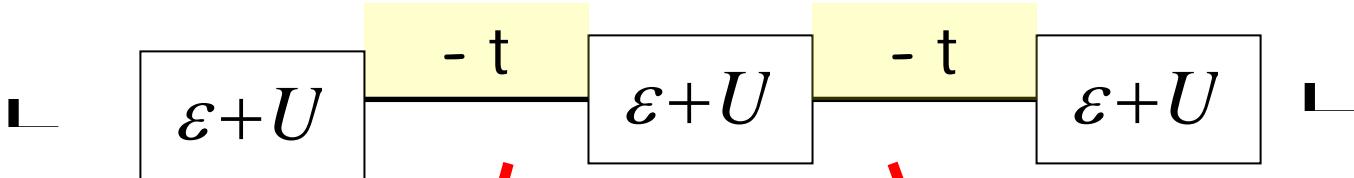
$$\Sigma_2(E) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & ** \end{bmatrix}$$

$$H = \begin{bmatrix} \epsilon & -t & 0 \\ -t & \epsilon & -t \\ 0 & -t & \epsilon \end{bmatrix}$$

Tight-binding parameters



Including a potential



$$\begin{aligned} & \downarrow \quad \downarrow \quad \downarrow \\ -te^{-ika} + \varepsilon + U - te^{+ika} \end{aligned}$$

$$= \varepsilon + U - 2t \cos ka$$

$$\approx (\varepsilon + U - 2t) + t (ka)^2$$

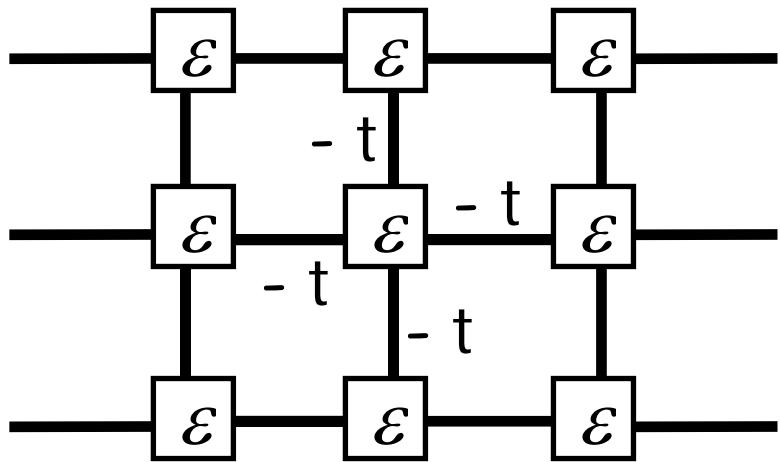
$$= E_c + U + \frac{\hbar^2}{2m} k^2$$

Including a vector potential

The diagram shows three rectangular boxes arranged horizontally. Each box contains the expression $\varepsilon + U$. Above the first and third boxes, there is a horizontal line connecting them, with the term $-te^{+i\alpha}$ placed above the line between the two boxes. Above the second and third boxes, there is another horizontal line connecting them, with the term $-te^{-i\alpha}$ placed above the line between the two boxes. Red arrows point downwards from each of these two horizontal lines to the corresponding terms in the mathematical derivation below.

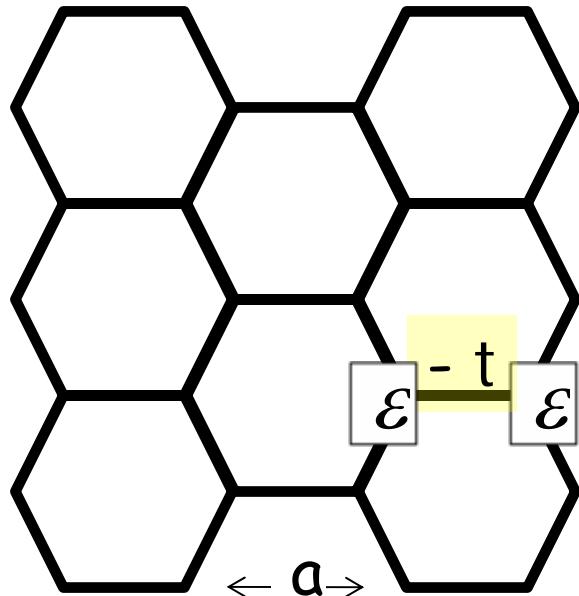
$$\begin{aligned} & -te^{+i\alpha} \quad -te^{-i\alpha} \\ & \downarrow \qquad \downarrow \qquad \downarrow \\ & -te^{+i\alpha} e^{-ika} + \varepsilon + U - te^{+ika} e^{-i\alpha} \\ & = \varepsilon + U - 2t \cos(ka - \alpha) \\ & \approx (\varepsilon + U - 2t) + t (ka - \alpha)^2 \\ & = E_c + U + \frac{\hbar^2}{2m} (k - qA/\hbar)^2 \end{aligned}$$

Tight-binding model (2-D square lattice)

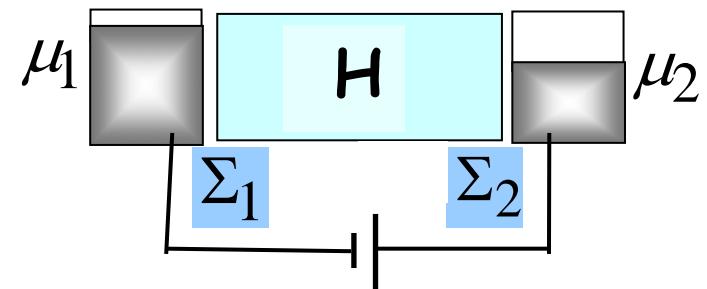
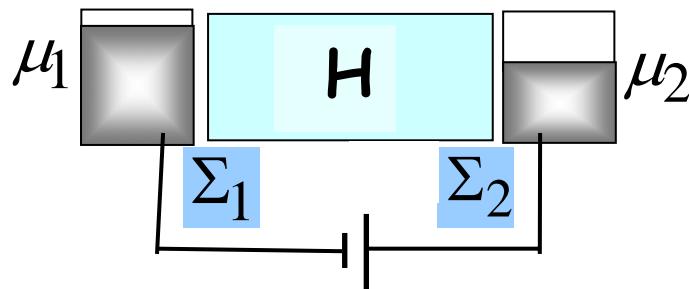
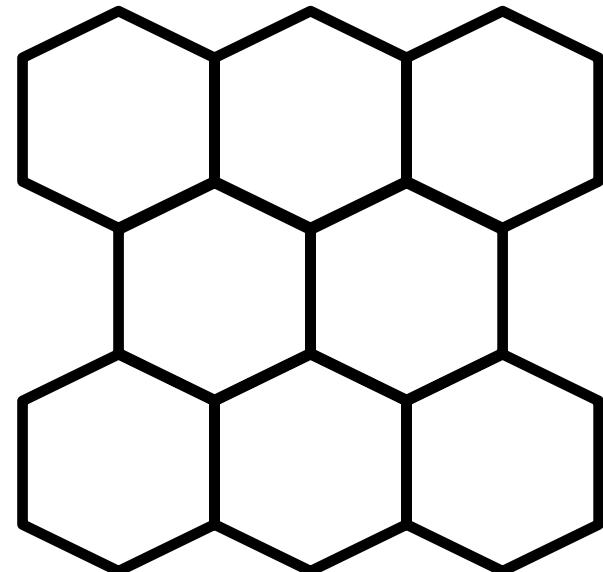


Tight-binding model (Graphene)

Armchair

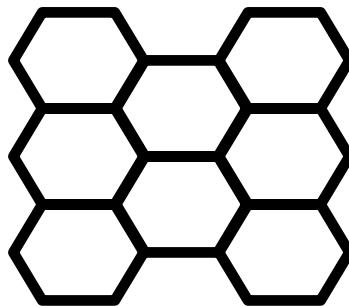


Zigzag

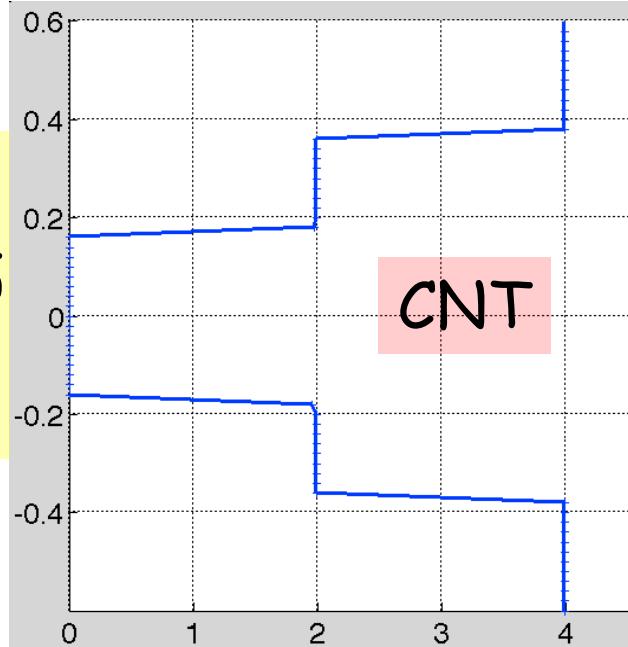


CNT versus Graphene

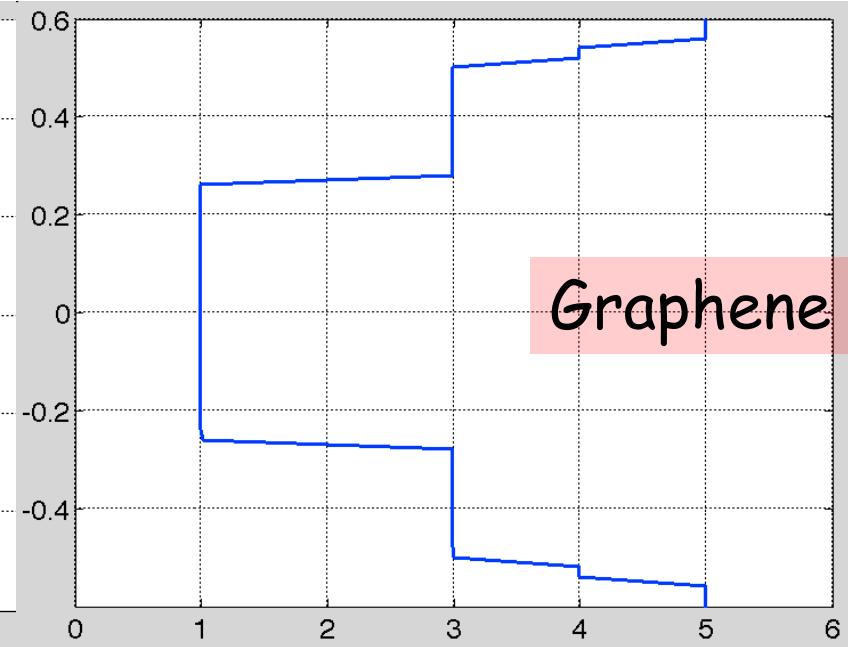
W ~
6 nm



Energy →



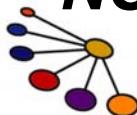
CNT



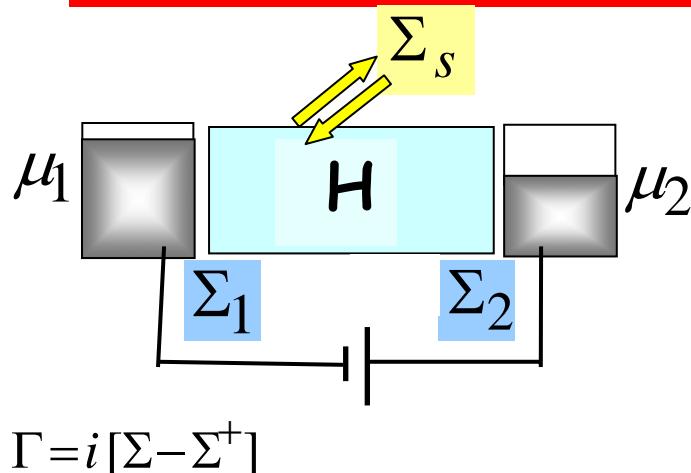
Graphene

Transmission →

NCN



** NEGF-Landauer equations



Green
function

$$[G] = [EI - H - \Sigma_1 - \Sigma_2 - \Sigma_s]^{-1}$$

"Density of states" $A = i[G - G^+]$

"Electron density"

$$G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1 + G\Sigma_s^{in} G^+$$

$$\varepsilon \rightarrow [H]$$

$$\gamma \rightarrow [\Gamma], [\Sigma]$$

$$n(E) \rightarrow [G^n(E)]$$

$$D(E) \rightarrow [A(E)]$$

Current

$$\frac{I_1}{q/\hbar} = \text{Trace} \left([\Gamma_1 A] f_1 - [\Gamma_1 G^n] \right)$$

Dephasing model: $[\Sigma_s^{in}] = D [G^n]$

NCN



Quantum Point Contacts: Experiment

VOLUME 60, NUMBER 9

PHYSICAL REVIEW LETTERS

29 FEBRUARY 1988

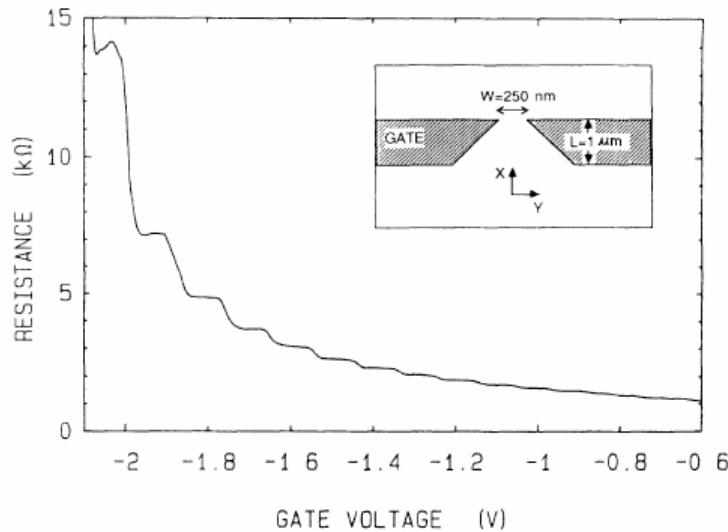


FIG. 1. Point-contact resistance as a function of gate voltage at 0.6 K. Inset: Point-contact layout.

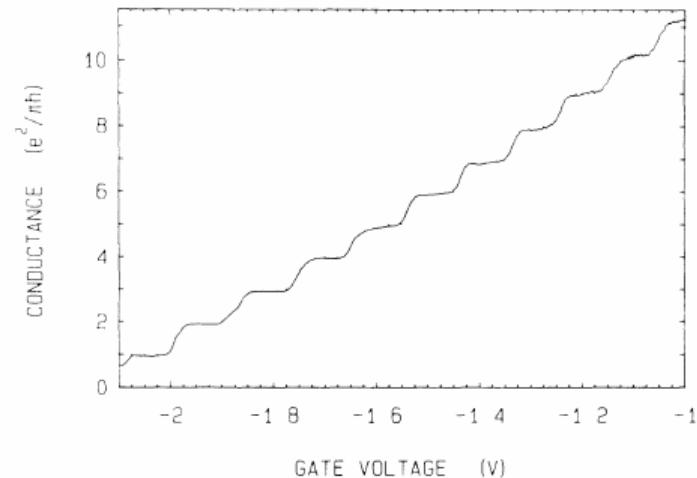


FIG. 2. Point-contact conductance as a function of gate voltage, obtained from the data of Fig. 1 after subtraction of the lead resistance. The conductance shows plateaus at multiples of $e^2/\pi\hbar$.

Also,

J. Phys. C: Solid State Phys. **21** (1988) L209–L214. Printed in the UK

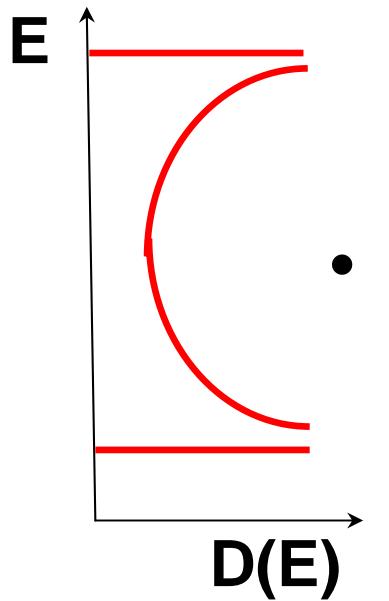
LETTER TO THE EDITOR

$$G \sim \frac{2}{3} \left(\frac{q^2}{2\pi} \right) M$$

for spin
1/25.8 KΩ



Number of modes in a 1D channel

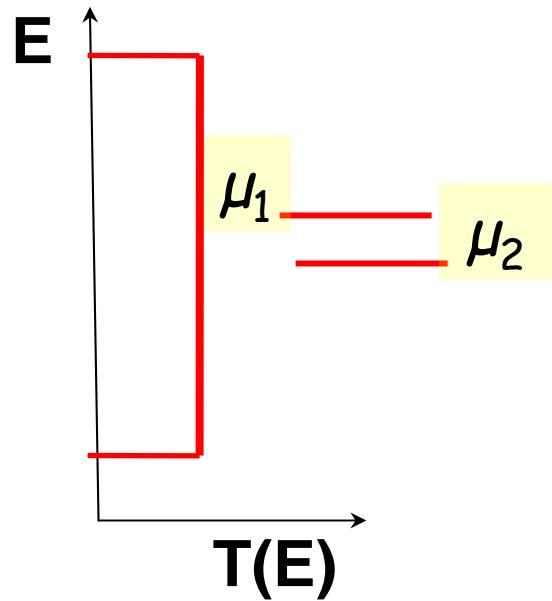


1-D

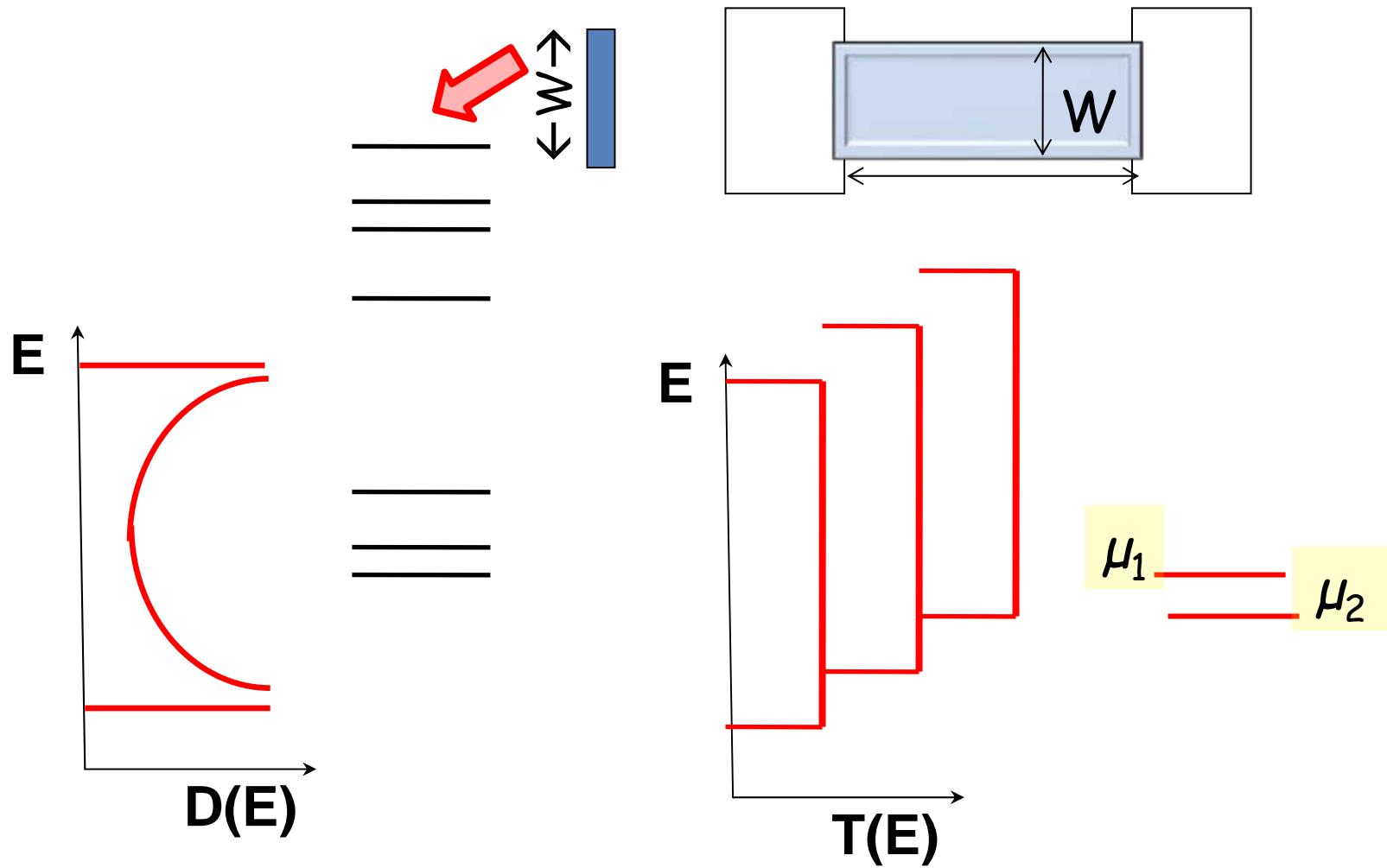
$$D = \frac{L}{\pi h\nu}$$



$$M = \pi D \gamma = \frac{\pi D h \nu}{L} = 1$$



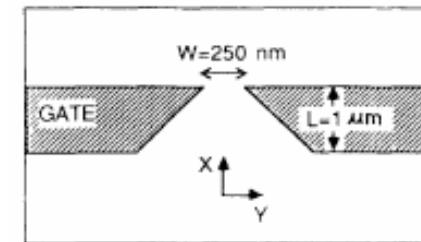
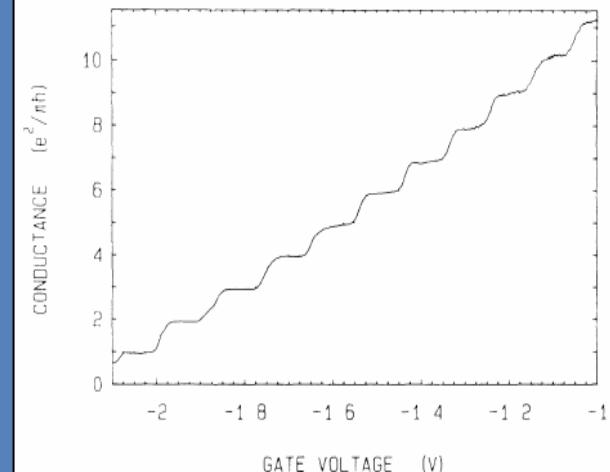
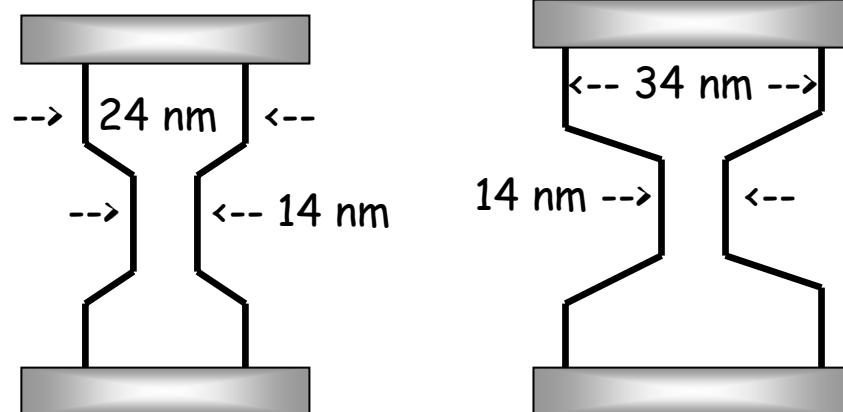
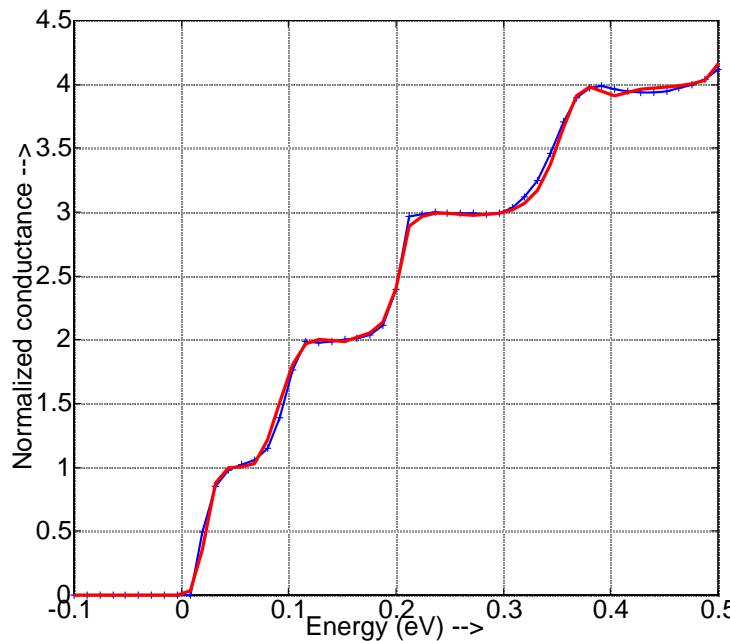
Number of modes in a 2D channel



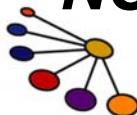
Quantum Point Contacts

Theory

Experiment



NCN



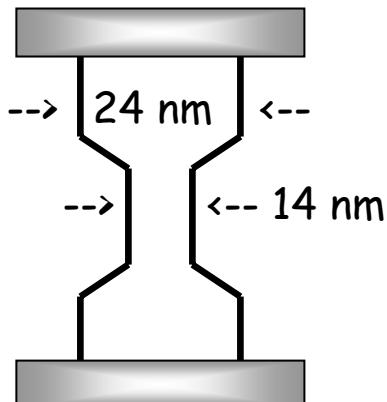
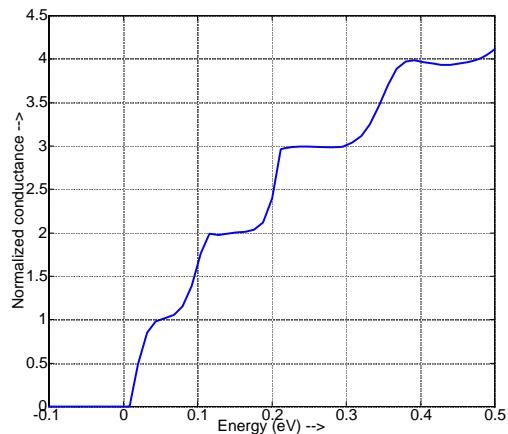
<http://www.nanohub.org/courses/cqt>

Supriyo Datta

PURDUE
UNIVERSITY

Can the numerical precede the physical ?

Numerical

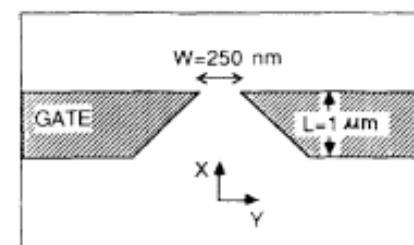
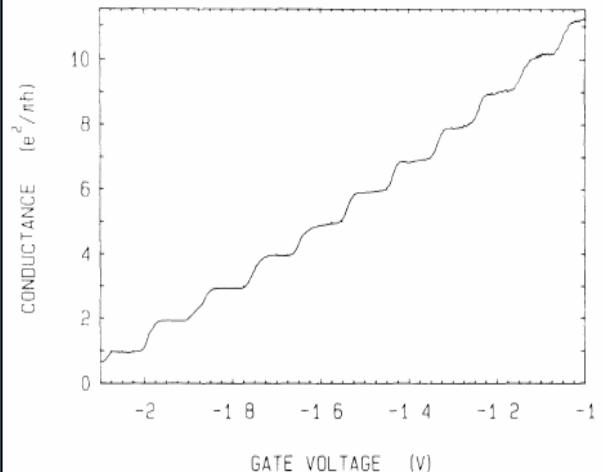


In 1988

Computers
were far less
powerful

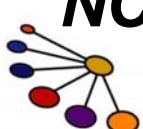
Theory
was far less
established

Physical

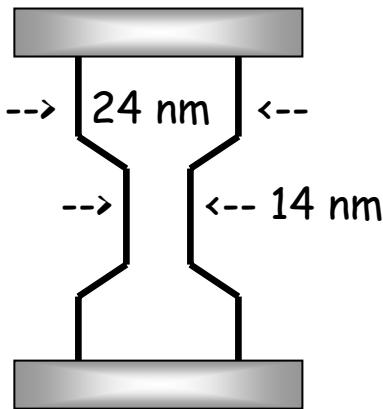
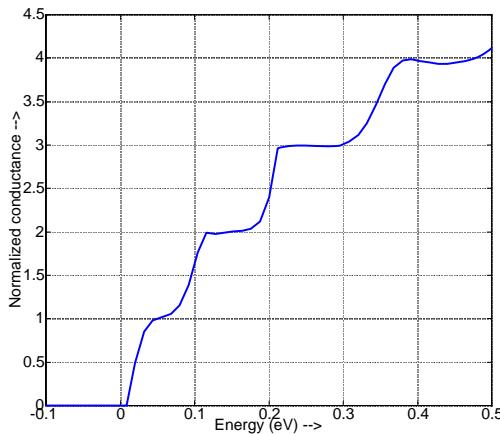


$$G = \frac{2}{\text{for spin}} \left(\frac{q^2}{2} \right) M \frac{1}{25.8 K\Omega}$$

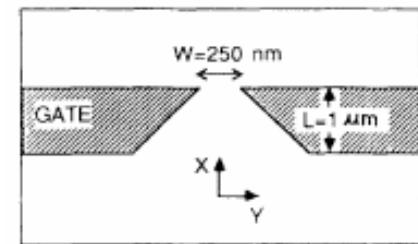
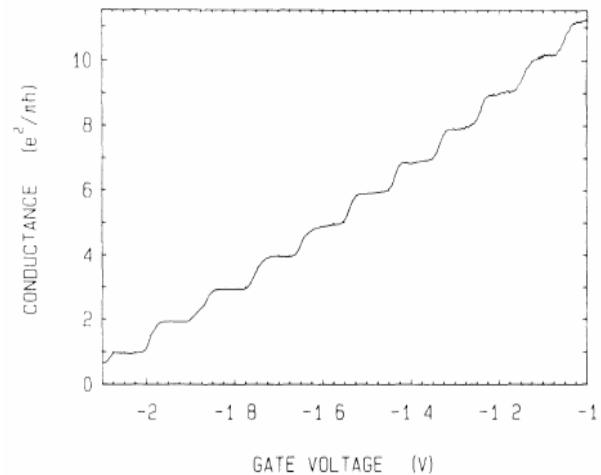
NCN



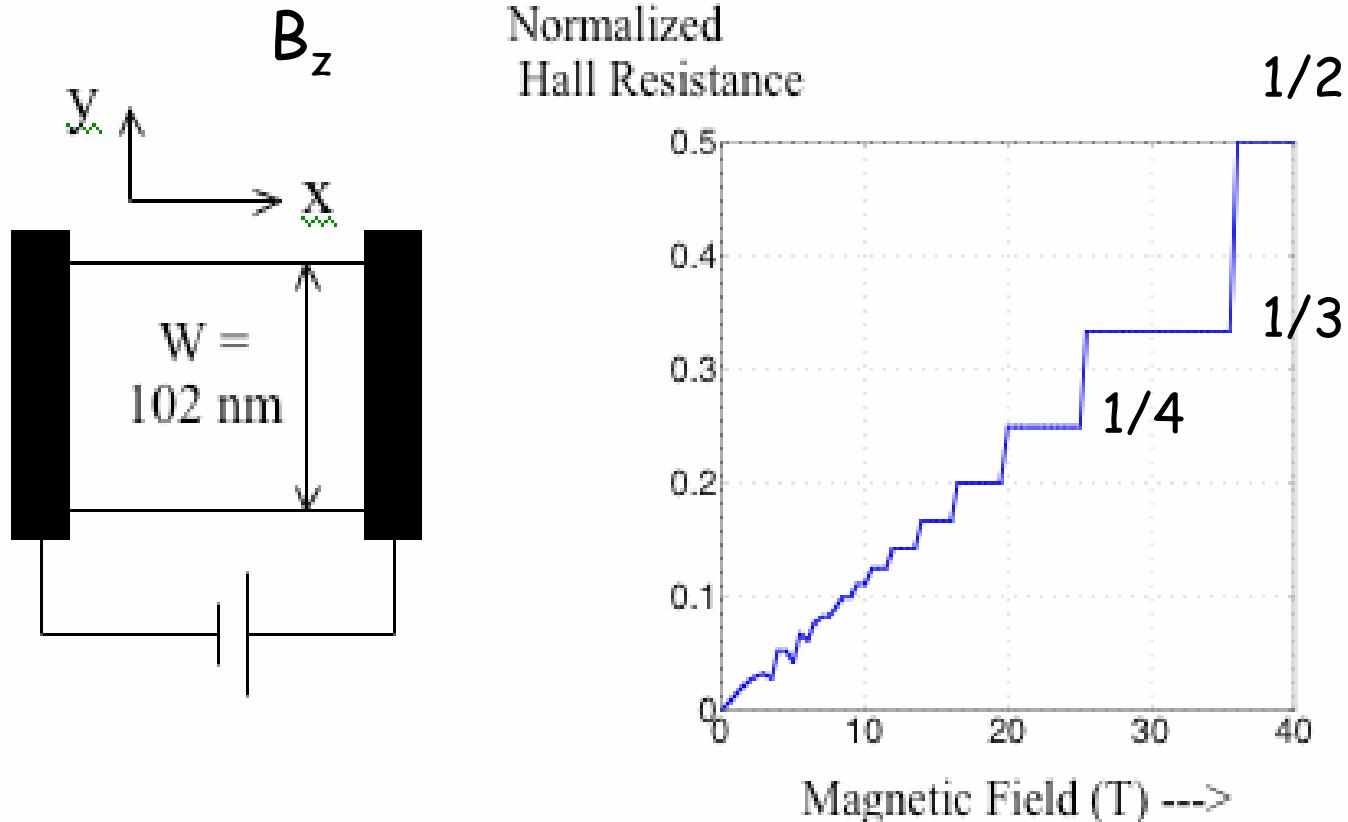
For the numerical to precede the physical



Numerical
experiments
have to be
Reproducible
Robust

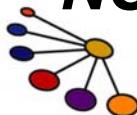
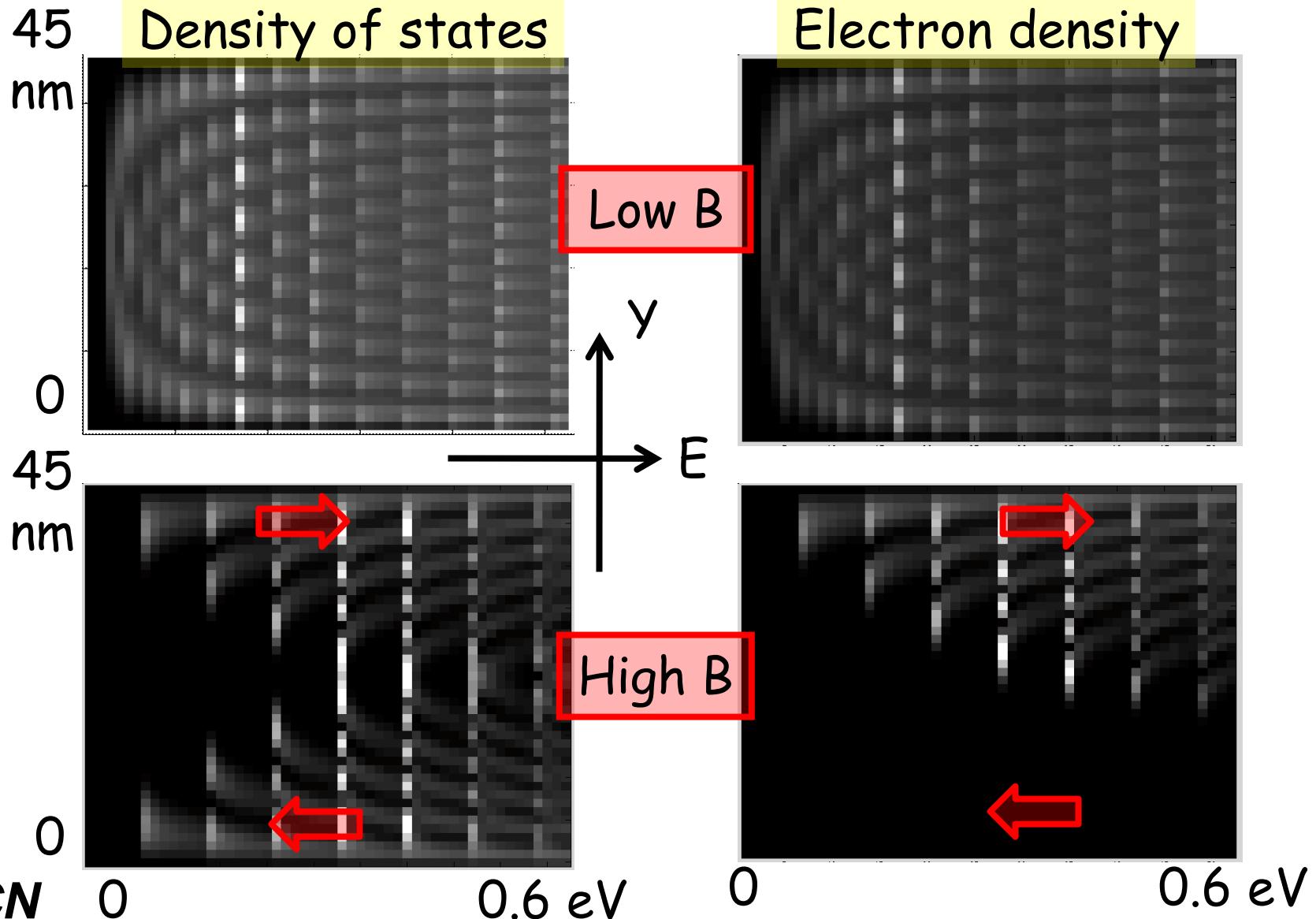


Hall Resistance

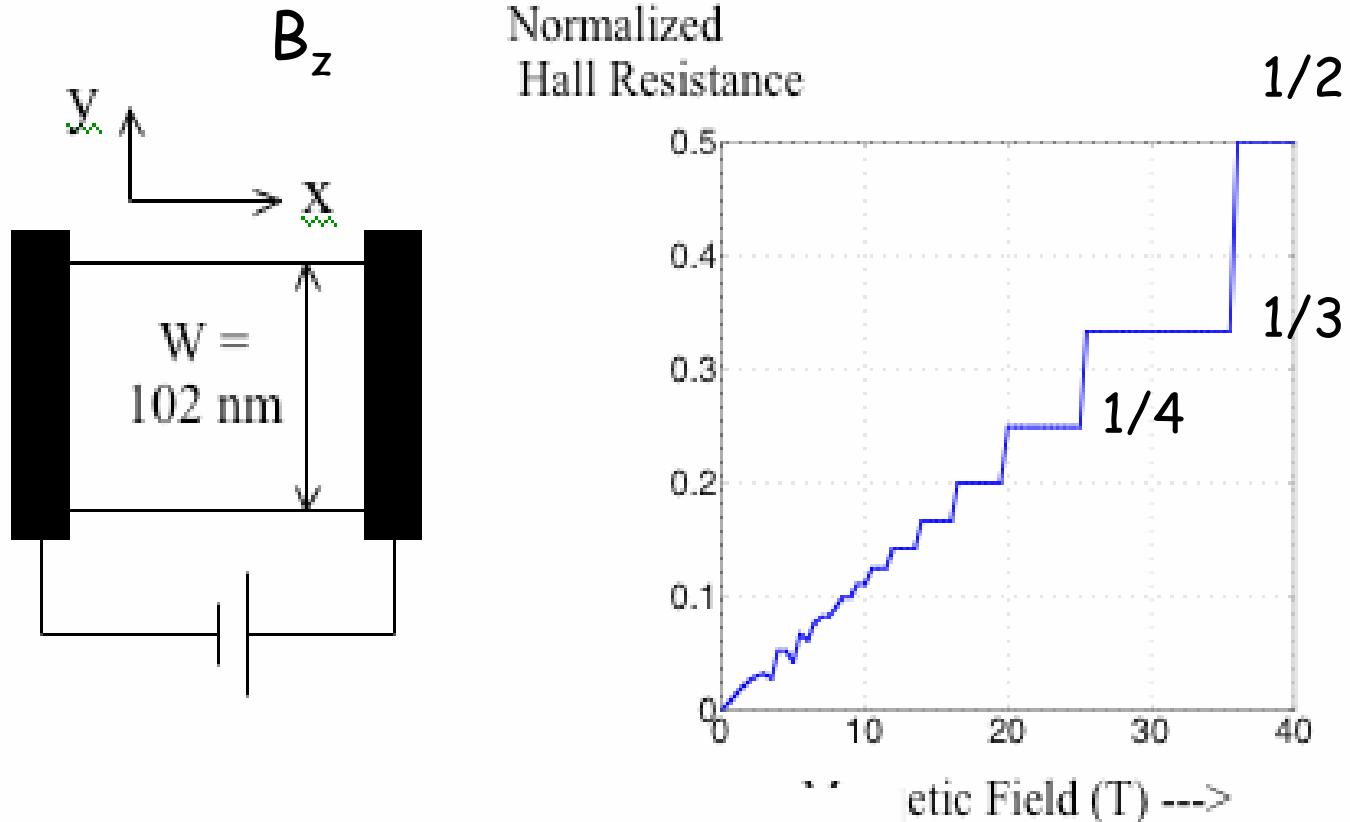


$$R = \left(\frac{h}{4e^2} \right) \frac{1}{M} \quad 25.8 \text{ K}\Omega/2$$

Edge state formation at high B-fields



Hall Resistance



VOLUME 45, NUMBER 6

PHYSICAL REVIEW LETTERS

11 AUGUST 1980

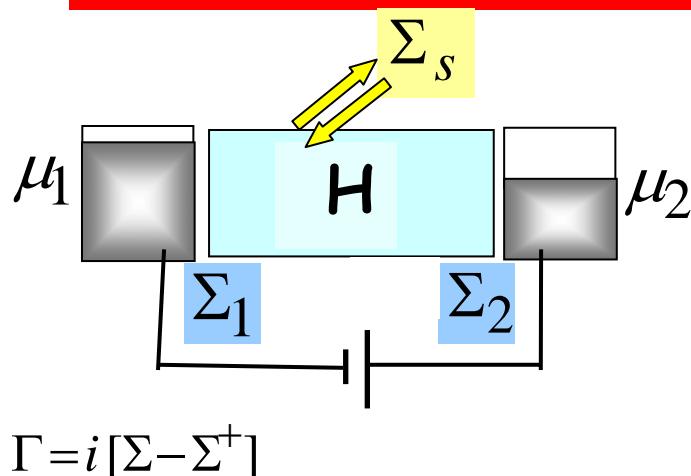
New Method for High-Accuracy Determination of the Fine-Structure Constant
Based on Quantized Hall Resistance

von Klitzing, Dorda and Pepper

$$R = \left(\frac{h}{4e^2} \right) \frac{1}{M} \quad 25.8 \text{ K}\Omega/2$$



NEGF-Landauer equations



Green
function

$$[G] = [EI - H - \Sigma_1 - \Sigma_2 - \Sigma_s]^{-1}$$

"Density of states" $A = i[G - G^+]$

"Electron density"

$$G^n = G\Gamma_2 G^+ f_2 + G\Gamma_1 G^+ f_1 + G\Sigma_s^{in} G^+$$

Current

$$\frac{I_1}{q/\hbar} = \text{Trace} \left([\Gamma_1 A] f_1 - [\Gamma_1 G^n] \right)$$

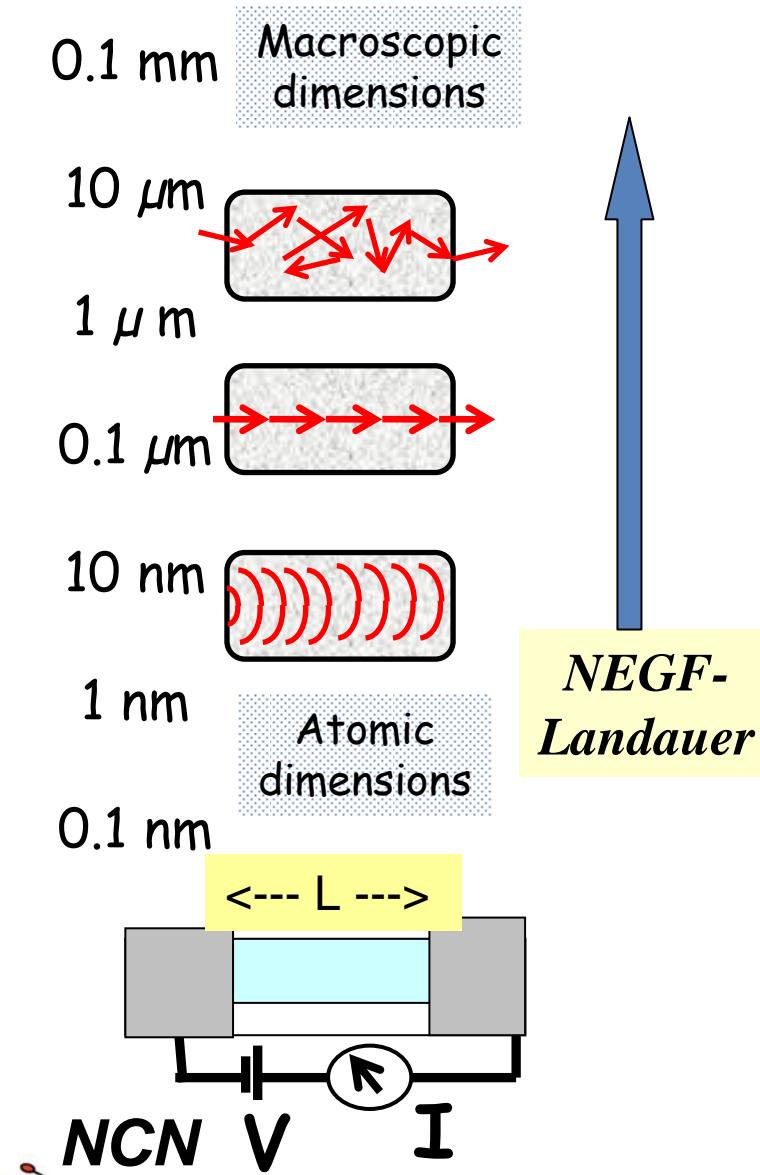
$$n(E) \rightarrow [G^n(E)]$$

$$D(E) \rightarrow [A(E)]$$

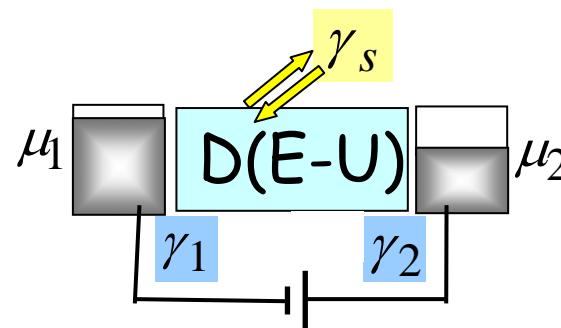
Dephasing model: $[\Sigma_s^{in}] = D [G^n]$



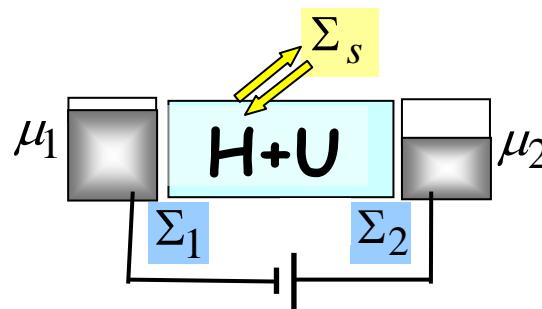
Nanoelectronics and the meaning of resistance



Lectures 1a,b:
Simple model



Lectures 3a,b:
Add spin



Lectures 2a,b:
Microscopic model



End of Lectures 2a,b