

NCN@Purdue - Intel Summer School: July 14-25, 2008

## **Physics of Nanoscale Transistors: Lecture 6:**

# **Quantum Transport in Nanoscale MOSFETS**

***Mark Lundstrom***

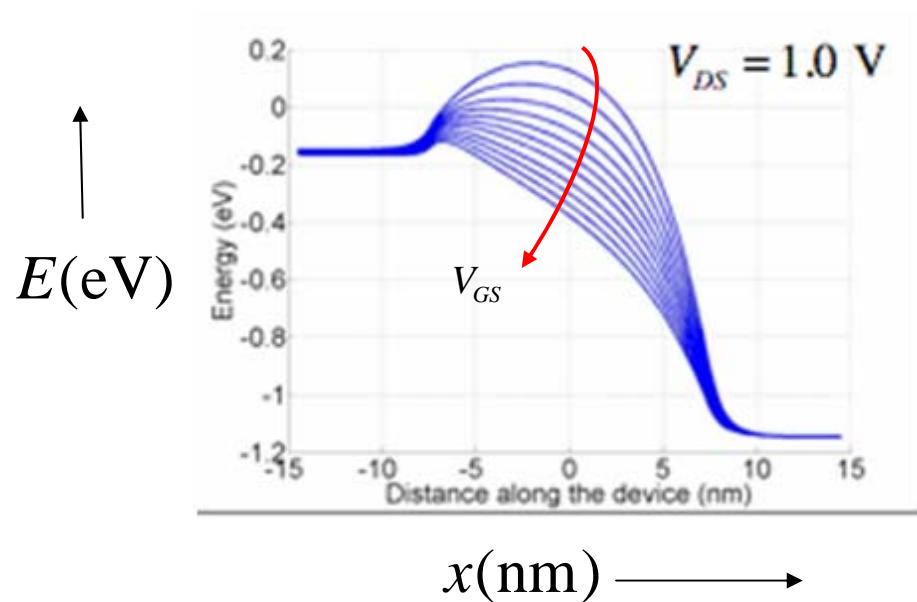
Network for Computational Nanotechnology  
Purdue University  
West Lafayette, Indiana USA

# outline

---

- 1) Introduction
- 2) A primer on ballistic quantum transport
- 3) Ballistic quantum transport in CNT MOSFETs
- 4) A primer on dissipative quantum transport
- 5) Dissipative quantum transport in CNT MOSFETs
- 6) Discussion
- 7) Summary

# physics of transistors



1) electrostatics

2) transport

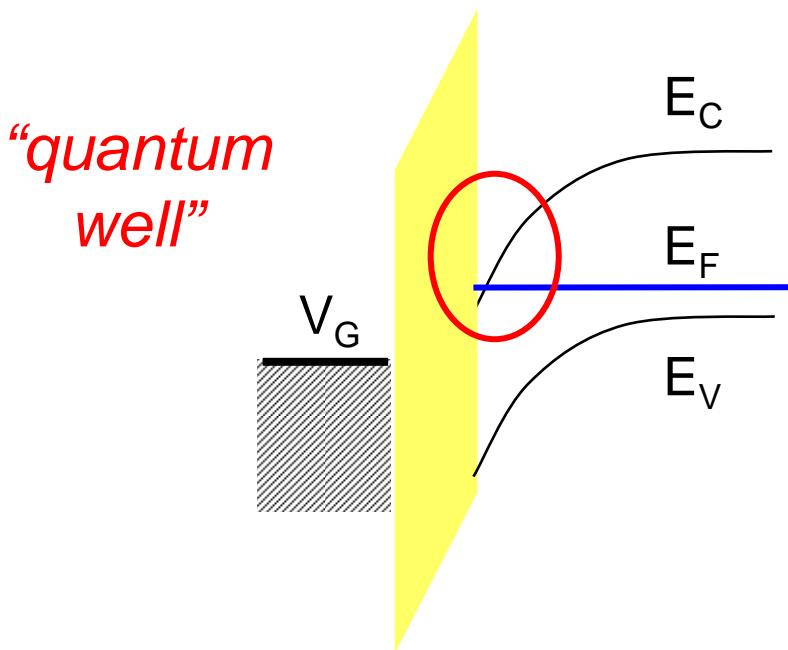
- semi-classical
  - drift-diffusion
  - Monte Carlo
  - .....
- **quantum**

# quantum mechanics and MOSFETs

---

- 1) Quantum confinement
- 2) Quantum transport

# quantum confinement in an MOS-C



$$\psi \sim e^{ikx}$$

$$p = \hbar k = \hbar \frac{2\pi}{\lambda}$$

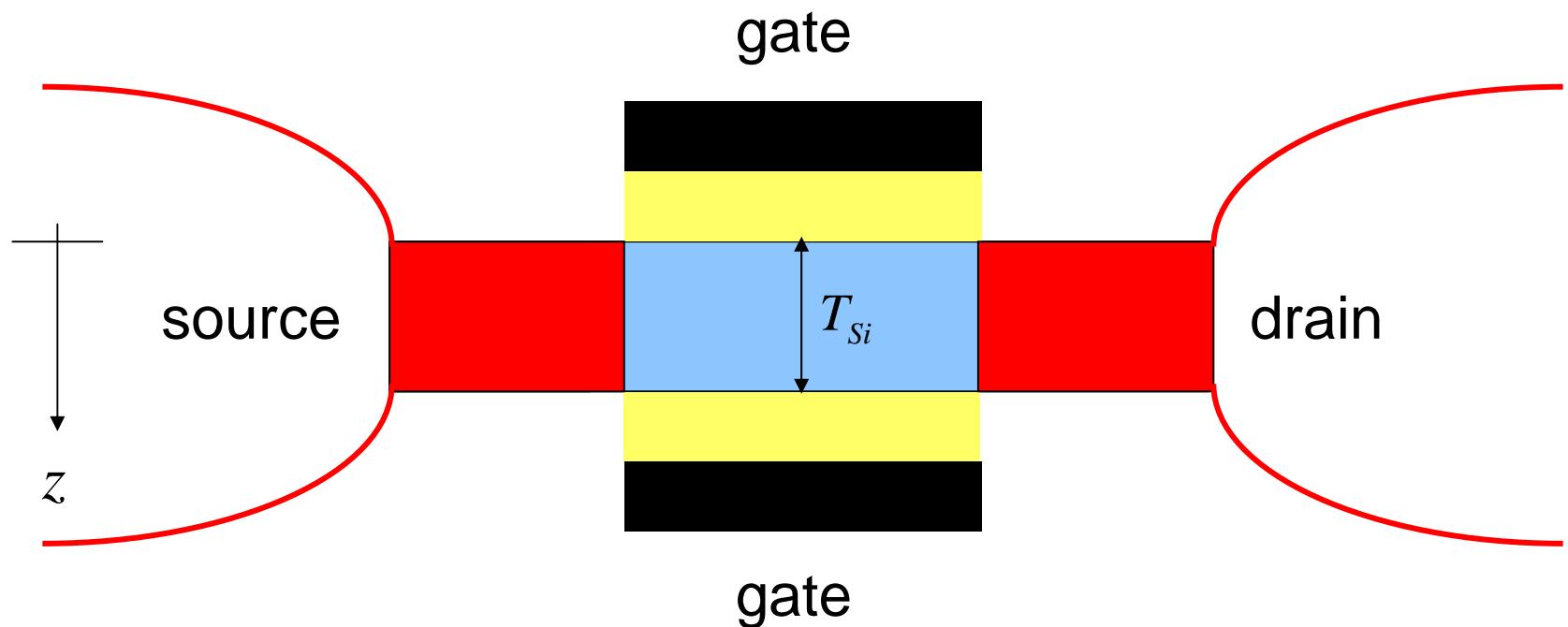
$$E = \frac{p^2}{2m^*}$$

$$\langle E \rangle = \frac{\langle p^2 \rangle}{2m^*} = \frac{3}{2} k_B T$$

$$\lambda_B = \frac{\hbar}{\sqrt{3m^* k_B T}} ; \text{ 10 nm (Si)}$$

# quantum confinement in UTB MOSFETs

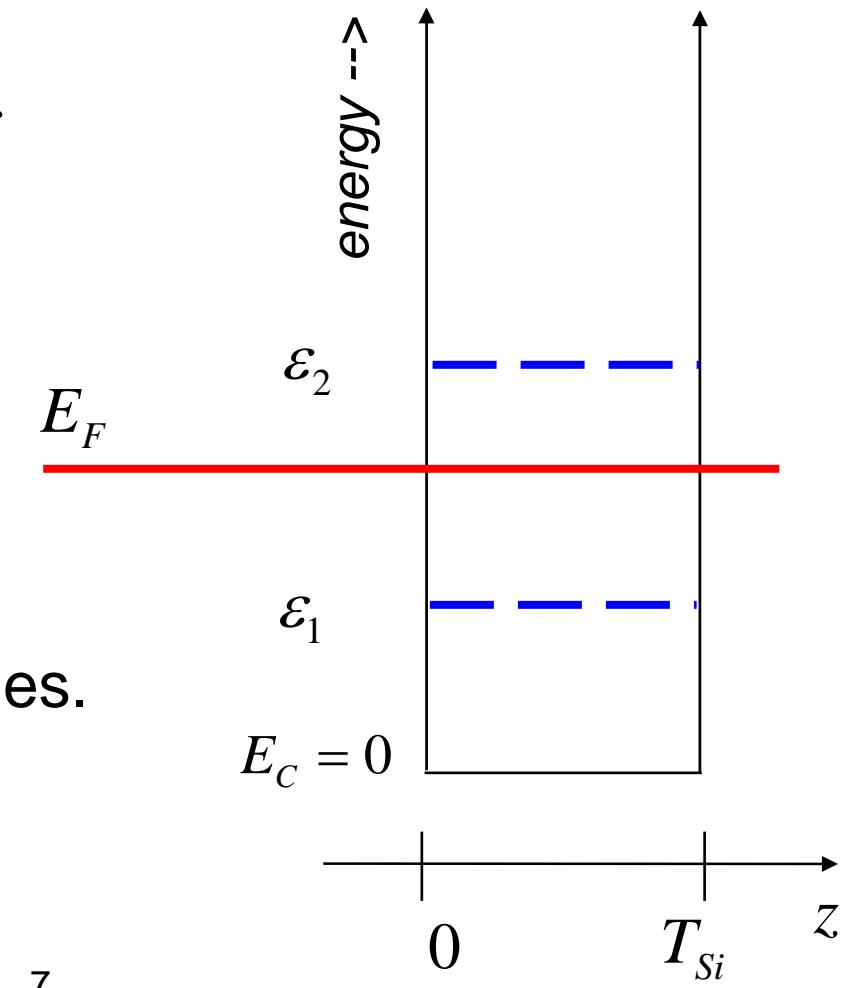
---



# energy levels (subbands)

$$\varepsilon_n = \frac{\hbar^2 n^2 \pi^2}{2m^* T_{Si}^2} \quad n = 1, 2, 3\dots$$

A light mass or narrow width  
leads to high subband energies.



# QM shift of the threshold voltage

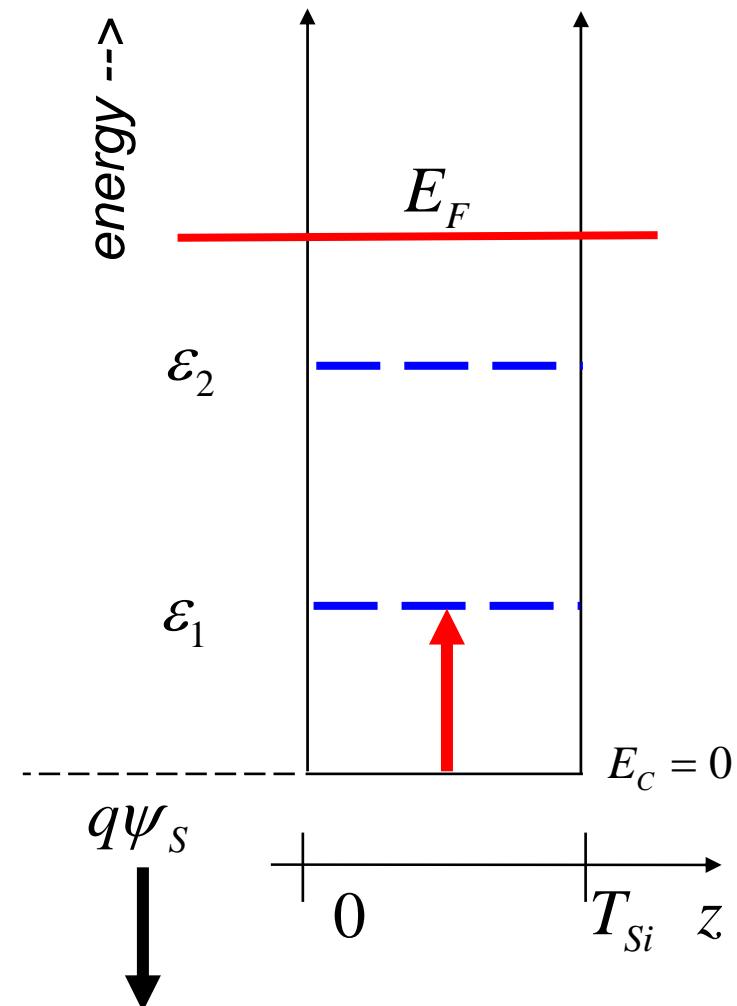
- to first order, QM simply raises  $E_C$  by  $\varepsilon_1$
- $\psi_S$  must increase by  $\Delta\psi_S^{QM}$  to achieve inversion

$$\psi_S = 2\psi_B$$

$\Rightarrow$

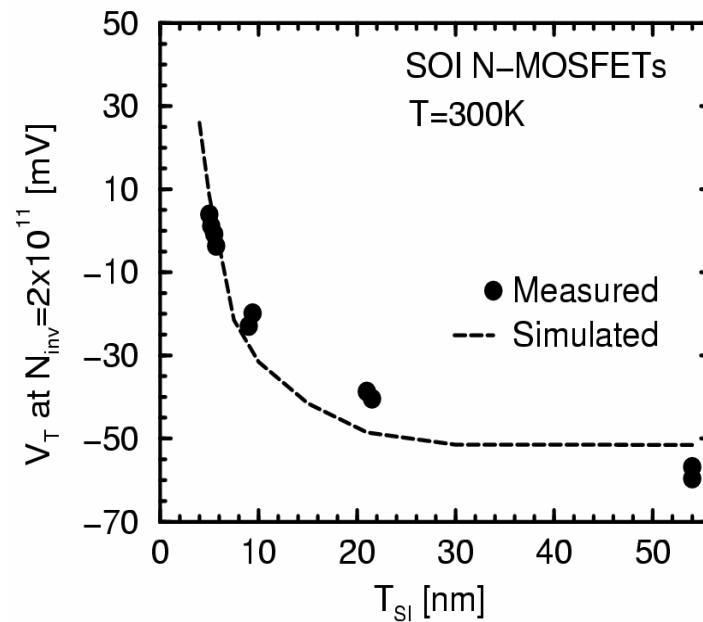
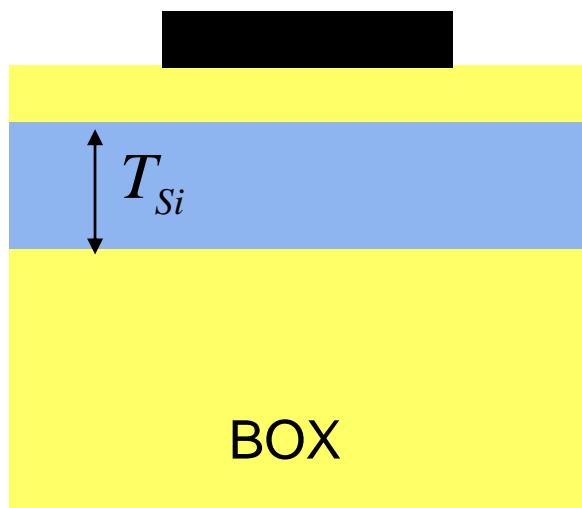
$$\psi_S = 2\psi_B + \Delta\psi_S^{QM}$$

$$\Delta\psi_S^{QM} ; \quad \varepsilon_1 / q$$



# QM shift of $V_T$ (experimental)

SOI



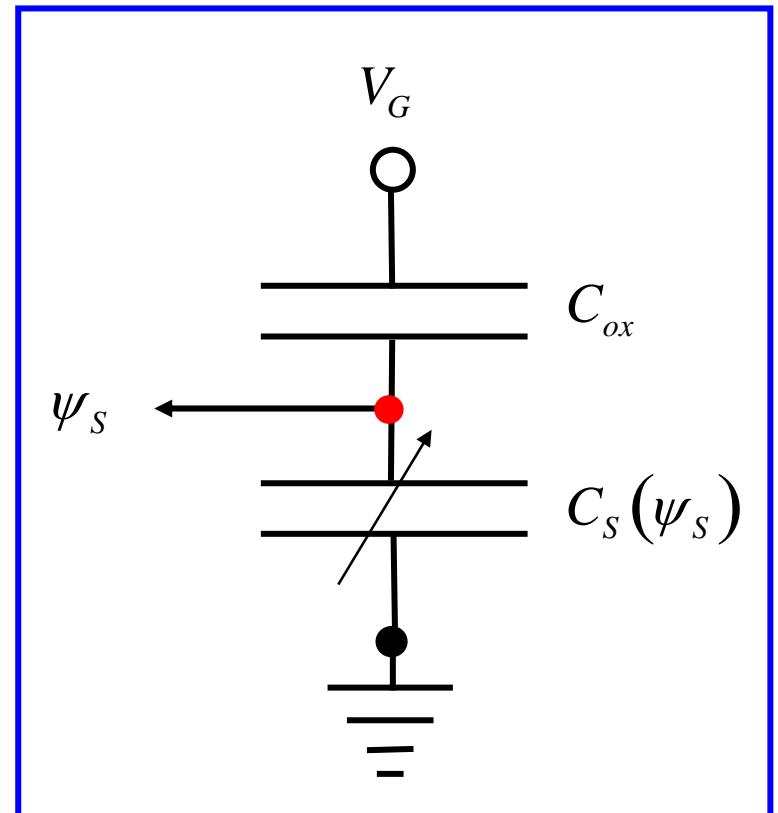
(D. Esseni *et al.* IEDM 2000 and TED 2001)

# influence of QM on $C_S$

$$C_S \equiv \frac{\partial(-Q_i)}{\partial \psi_S}$$

$$C_G = \frac{C_{ox} C_S}{C_{ox} + C_S} < C_{ox}$$

$C_S(\text{QM}) < C_S(\text{classical})$



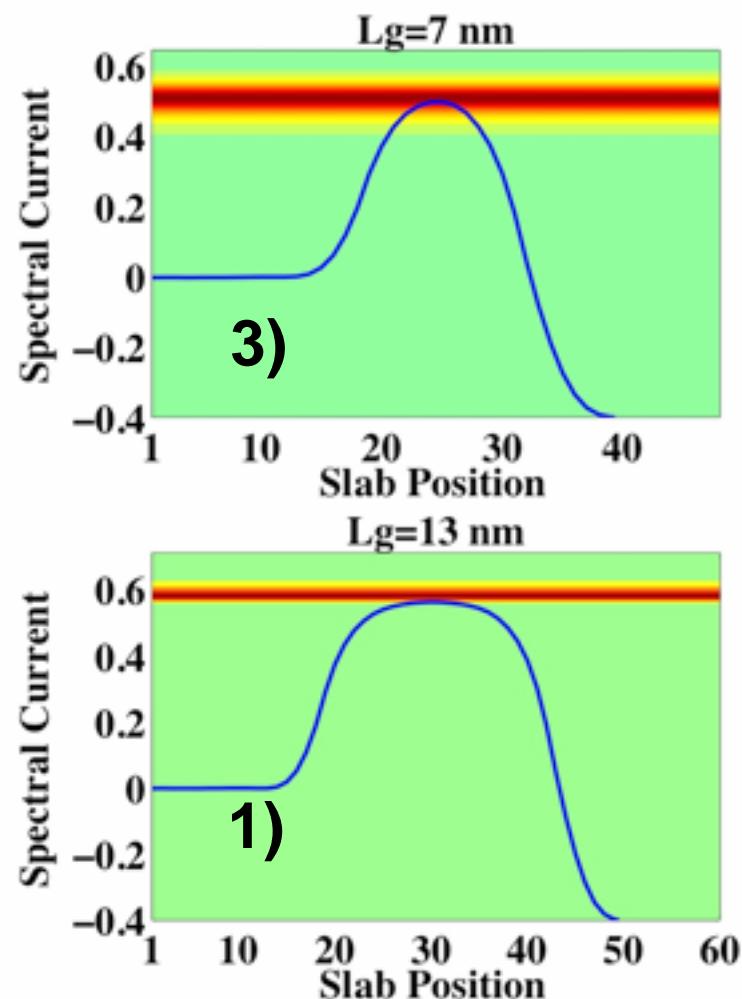
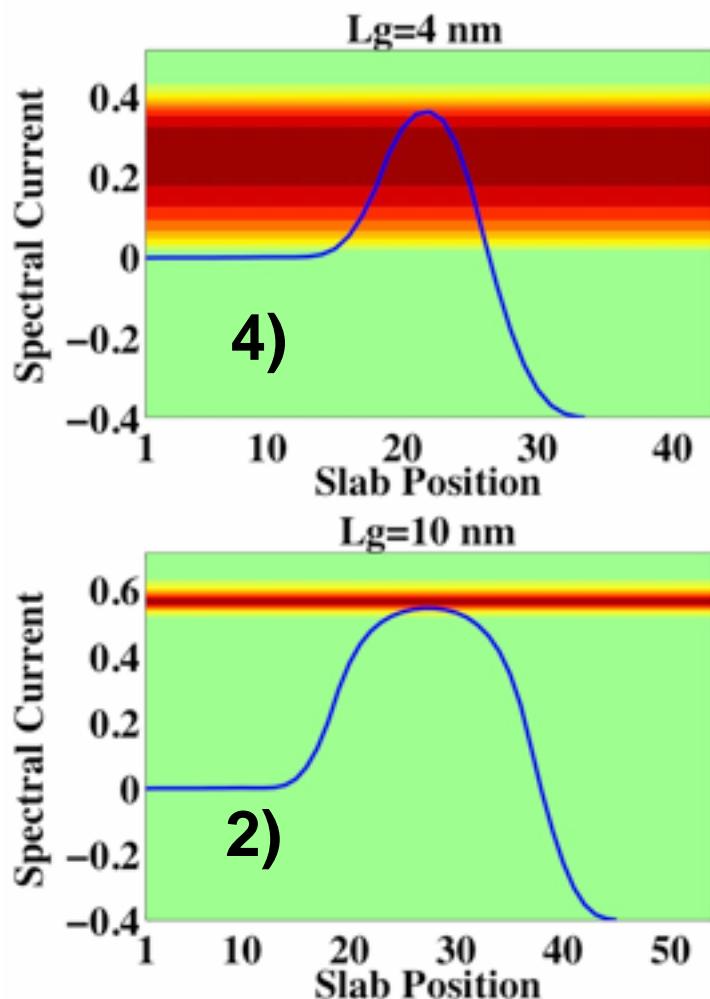
# QM and MOSFETs

---

## *Quantum mechanics:*

- 1) increases  $V_T$
- 2) decreases  $C_S$  (inv) and, therefore,  $C_G$ (on)
- 3) affects transport along the channel...

# S/D tunneling



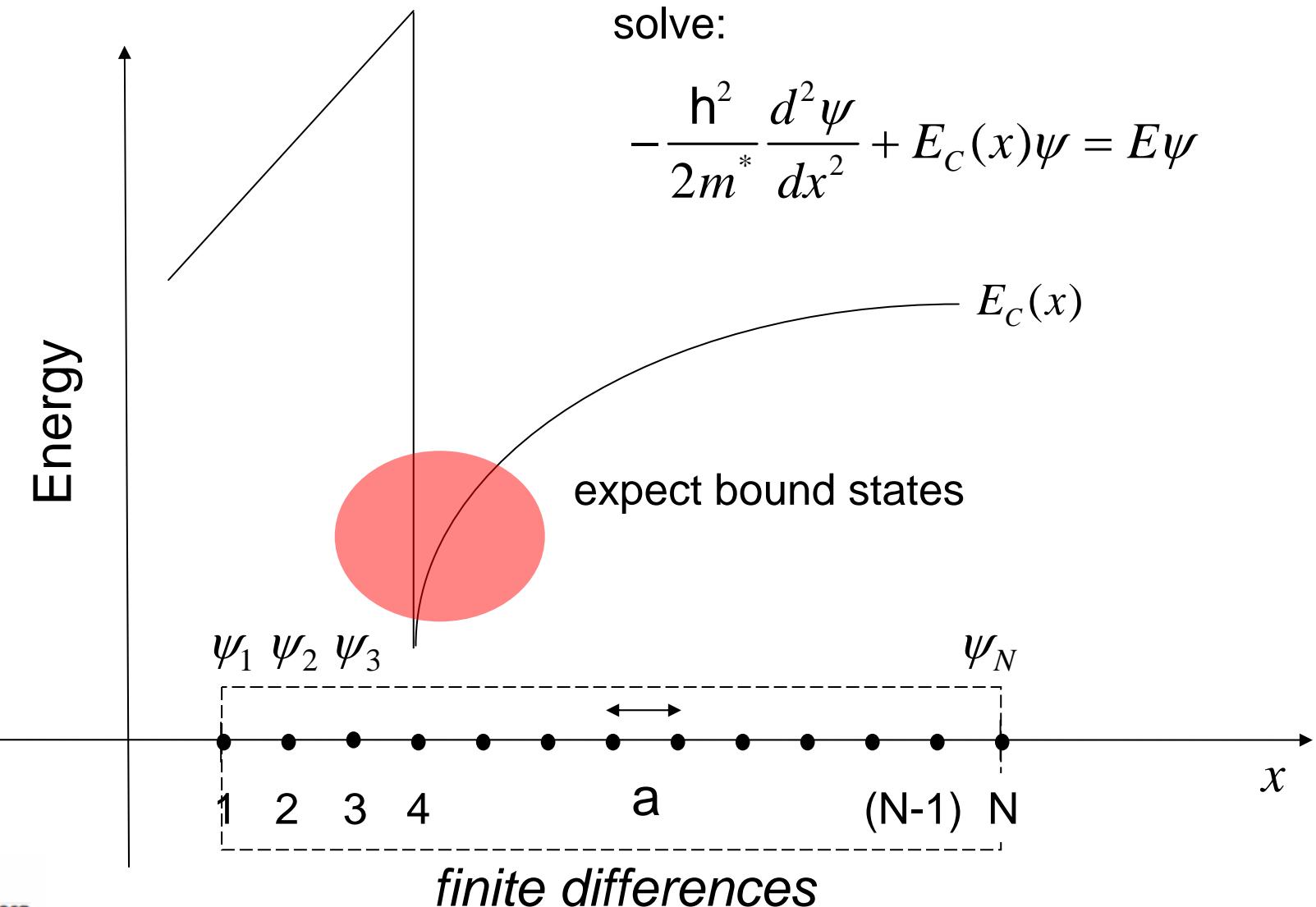
from M. Luisier, ETH Zurich

# outline

---

- 1) Introduction
- 2) A primer on ballistic quantum transport**
- 3) Ballistic quantum transport in CNT MOSFETs
- 4) A primer on dissipative quantum transport
- 5) Dissipative quantum transport in CNT MOSFETs
- 6) Discussion
- 7) Summary

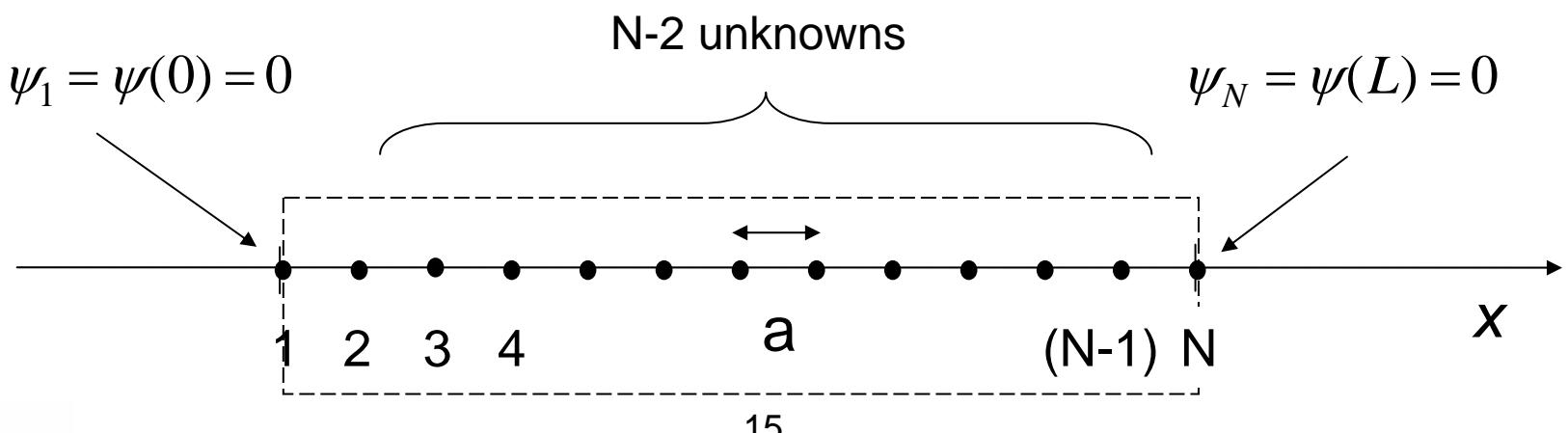
# solving the wave equation: bound states



# discretization

$$-\frac{\hbar^2}{2m^*} \frac{d^2\psi}{dx^2} + E_c(x)\psi = E\psi \quad \left. \frac{d^2\psi}{dx^2}\right|_i = \frac{\psi_{i-1} - 2\psi_i + \psi_{i+1}}{a^2}$$

$$[-t_0\psi_{i-1} + (2t_0 + E_{Ci})\psi_i - t_0\psi_{i+1}] = E\psi_i \quad i = 2, 3, \dots, N-1 \quad t_0 \equiv \frac{\hbar^2}{2m^* a^2}$$



# eigenvalue problem

---

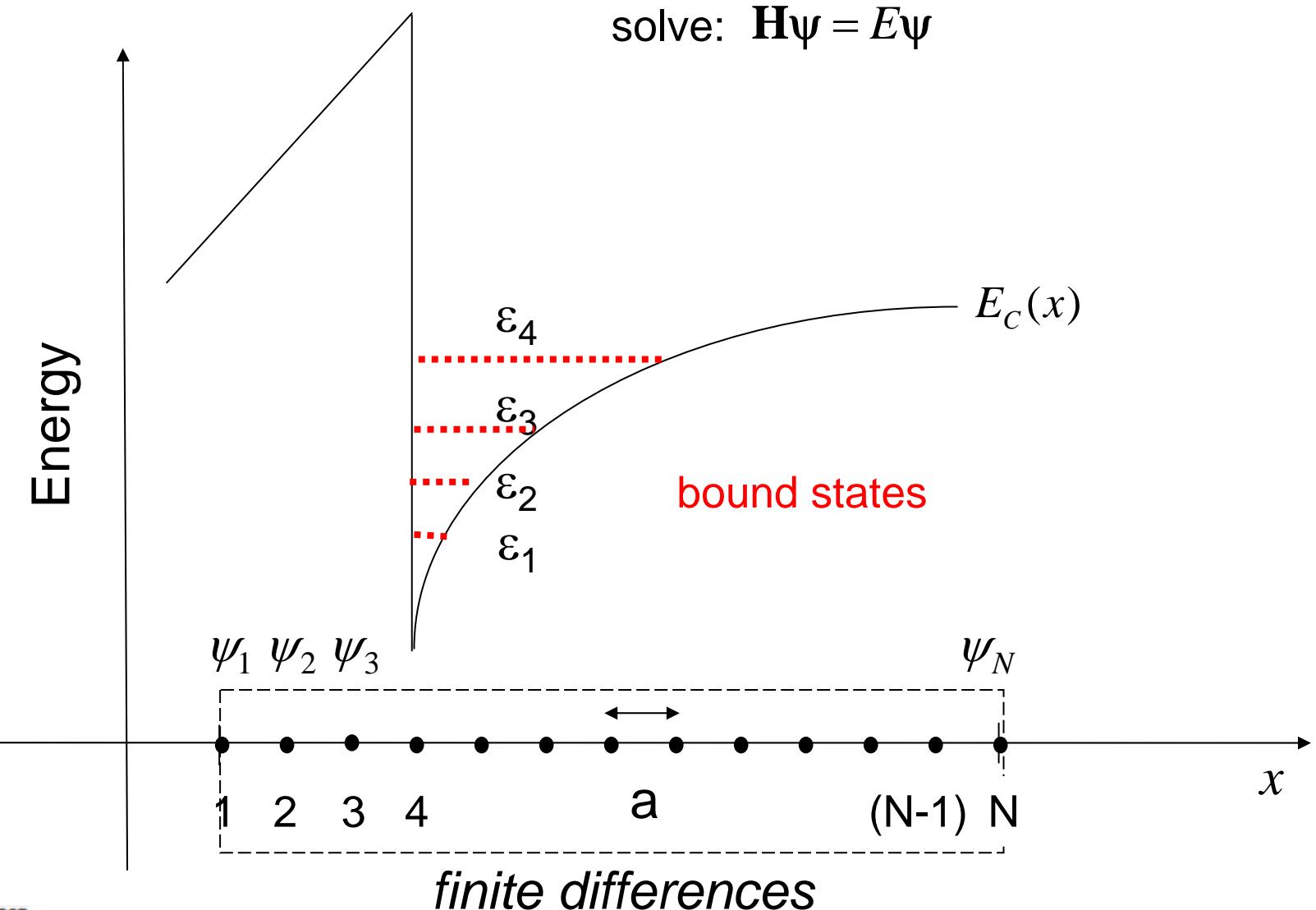
$$[-t_0\psi_{i-1} + (2t_0 + E_{Ci})\psi_i - t_0\psi_{i+1}] = E\psi_i \quad (i = 2, 3, \dots, N-1)$$

$$\mathbf{H}\psi = E\psi$$

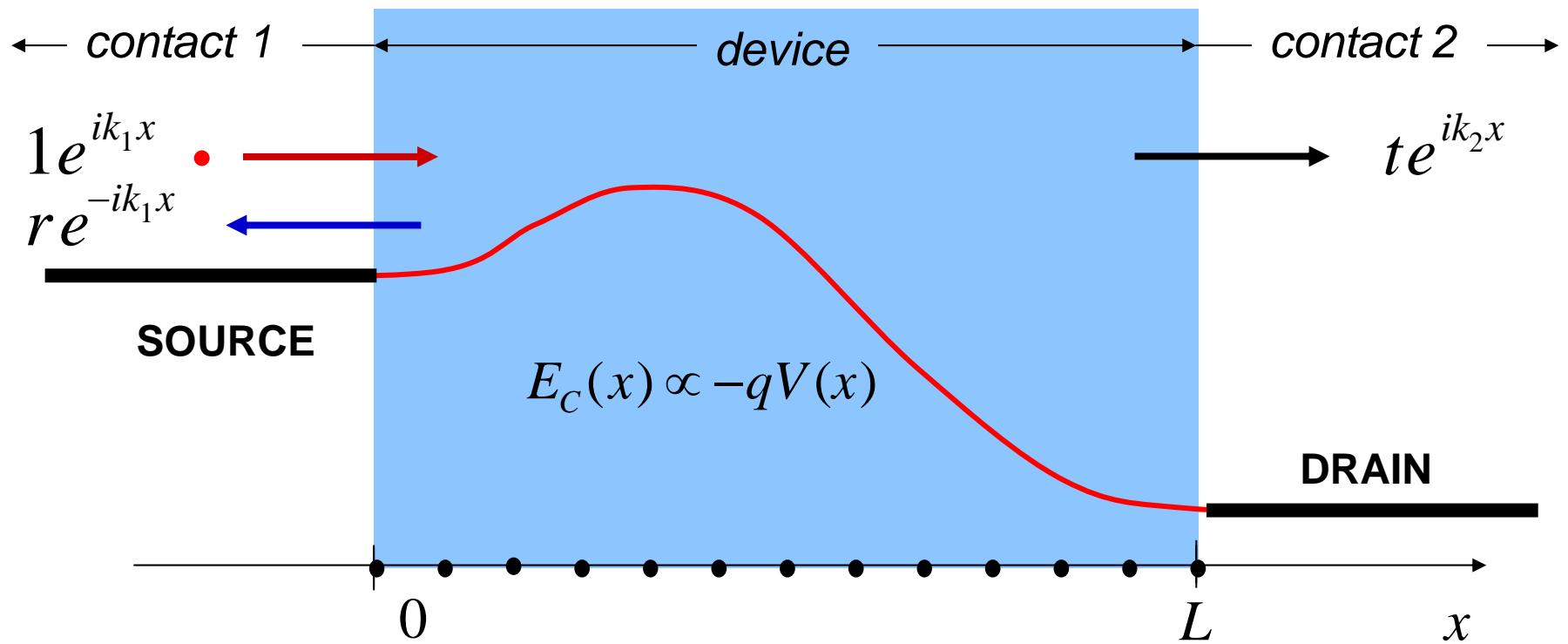
$$\begin{bmatrix} & & \\ -t_0 & (2t_0 + E_{C_2}) & -t_0 \\ & & \end{bmatrix} \begin{pmatrix} \psi_2 \\ \vdots \\ \psi_{N-1} \end{pmatrix} = E \begin{pmatrix} \psi_2 \\ \vdots \\ \psi_{N-1} \end{pmatrix}$$

$N-2 \times N-2 \quad (N-2) \times 1 \quad (N-2) \times 1$

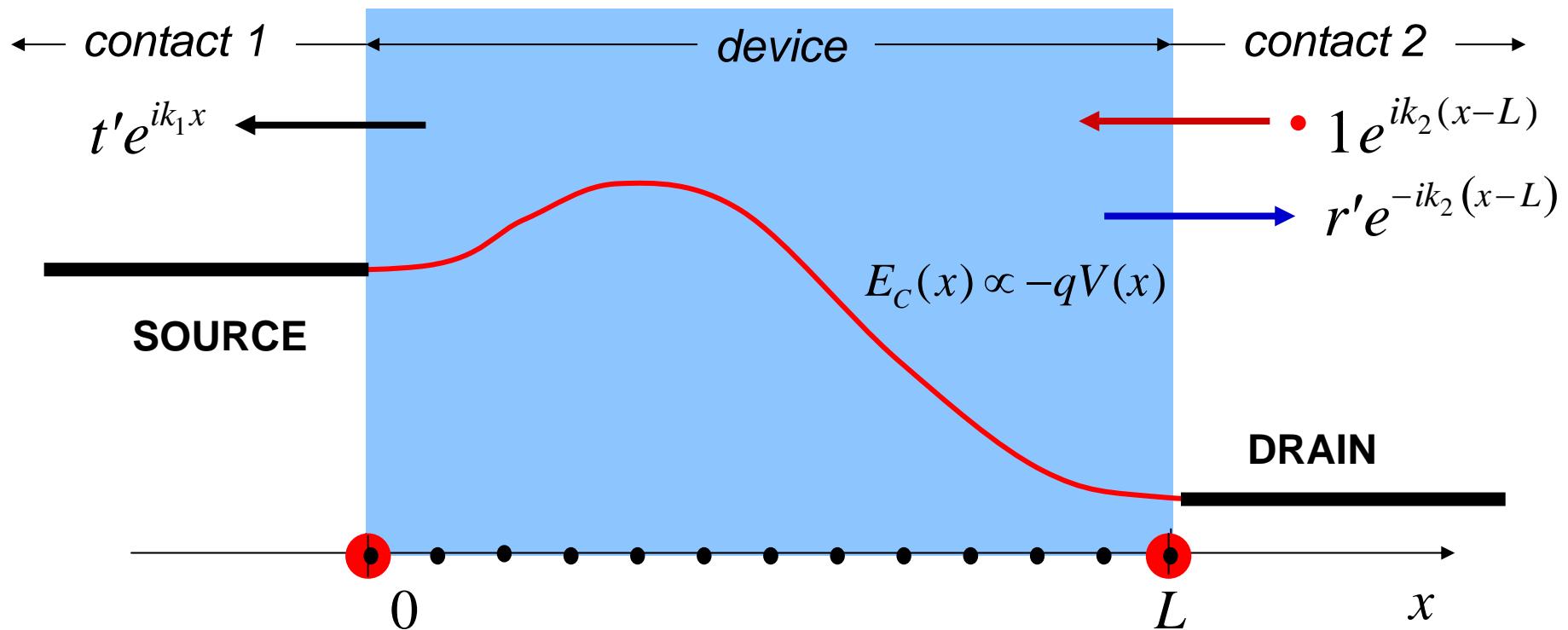
# eigenvalues: bound states



# open systems: source injection



# open systems: drain injection



$$E\psi_i - [-t_0\psi_{i-1} + (2t_0 + E_{Ci})\psi_i - t_0\psi_{i+1}] = 0 \quad i = 1, 2, 3, \dots$$

# open boundary conditions

---

$$E\psi_1 - [-t_0\psi_0 + (2t_0 + E_{C1})\psi_1 - t_0\psi_2] = 0 \quad (i=1)$$

$$\psi_0 = \frac{\psi_1 e^{ik_1 a} - (e^{ik_1 a} - e^{-ik_1 a})}{2}$$

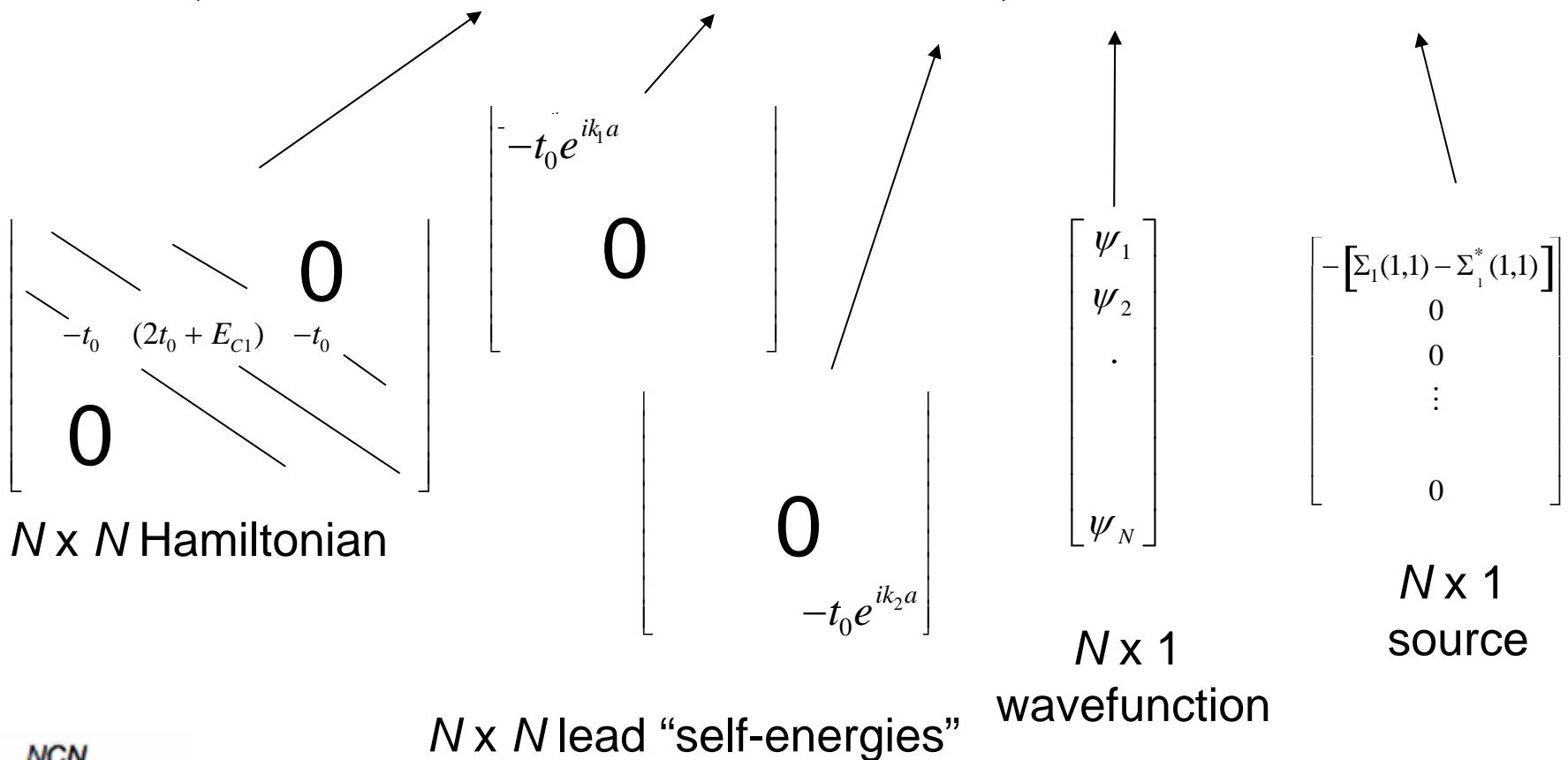
1)                    2)

To account for the open boundary condition at  $x = 0$ , we

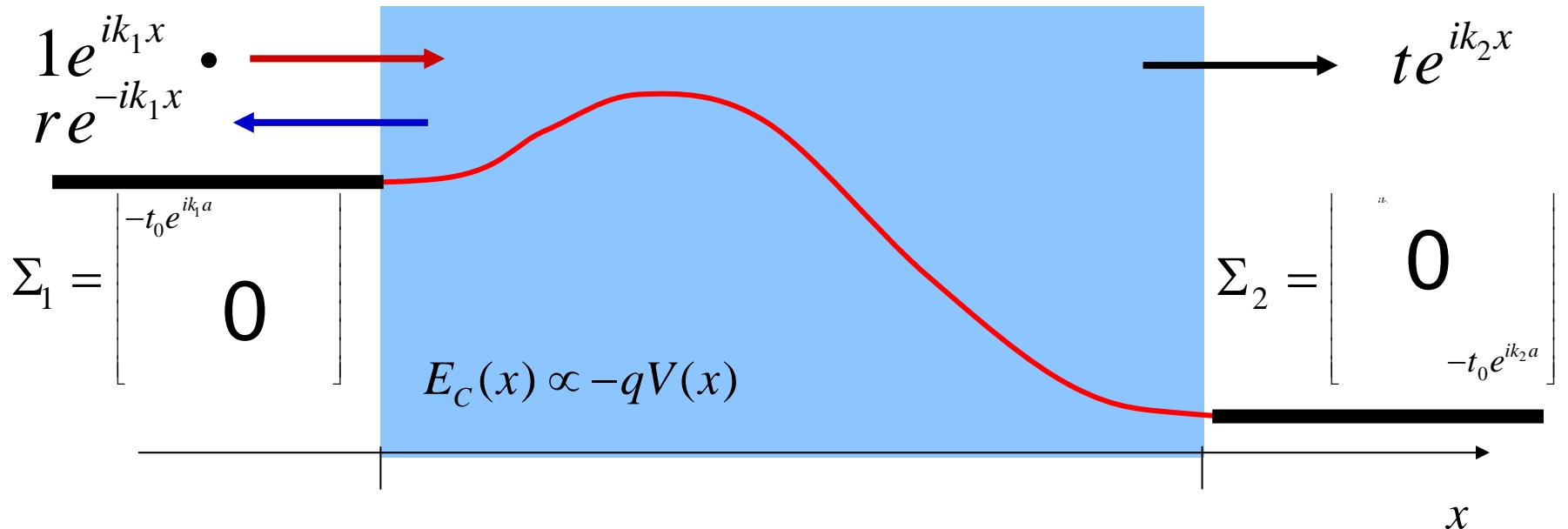
- 1) add  $-t_0 e^{ik_1 a}$  to the diagonal
- 2) add  $t_0 (e^{ik_1 a} - e^{-ik_1 a})$  to the first column of the RHS

# discretized wave equation

$$(E[I] - [H] - [\Sigma_1] - [\Sigma_2])\{\psi\} = \{S\}$$



## *a word about $E(k)$*

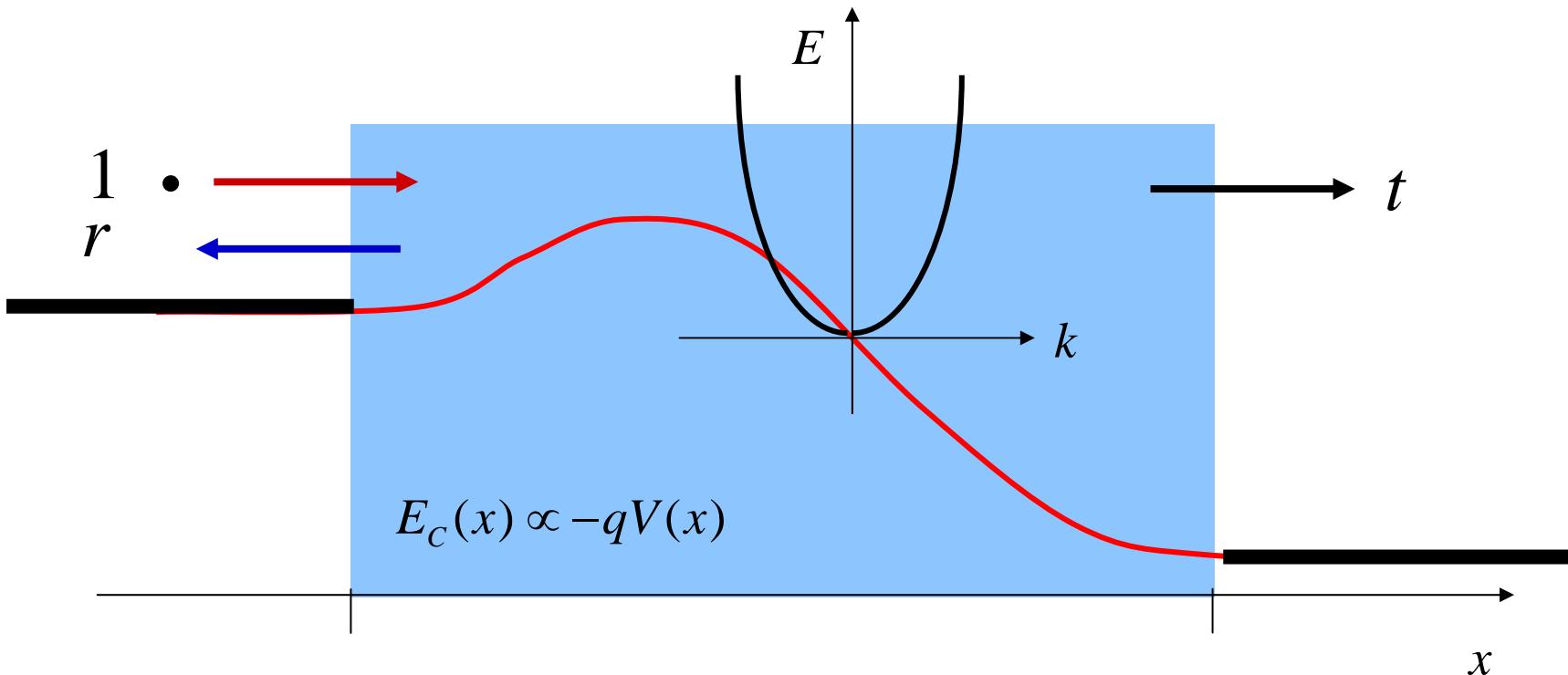


$E(k)$

***There is No  $E(k)$  in the device!***  
*( $k$  refers to the leads)*

$E(k)$

# semi-classical device analysis



semi-classical approach:

***Assumes an  $E(k)$  inside the device!***

“local density-of-states”

$$g_{1D}(x, E) = \frac{1}{\pi h} \sqrt{\frac{2m^*}{E - E_C(x)}}$$

# solving the wave equation

---

$$(E[I] - [H] - [\Sigma_1] - [\Sigma_2])\{\psi\} = \{S\}$$

(not an eigenvalue problem - energy is continuous)

*formal solution:*

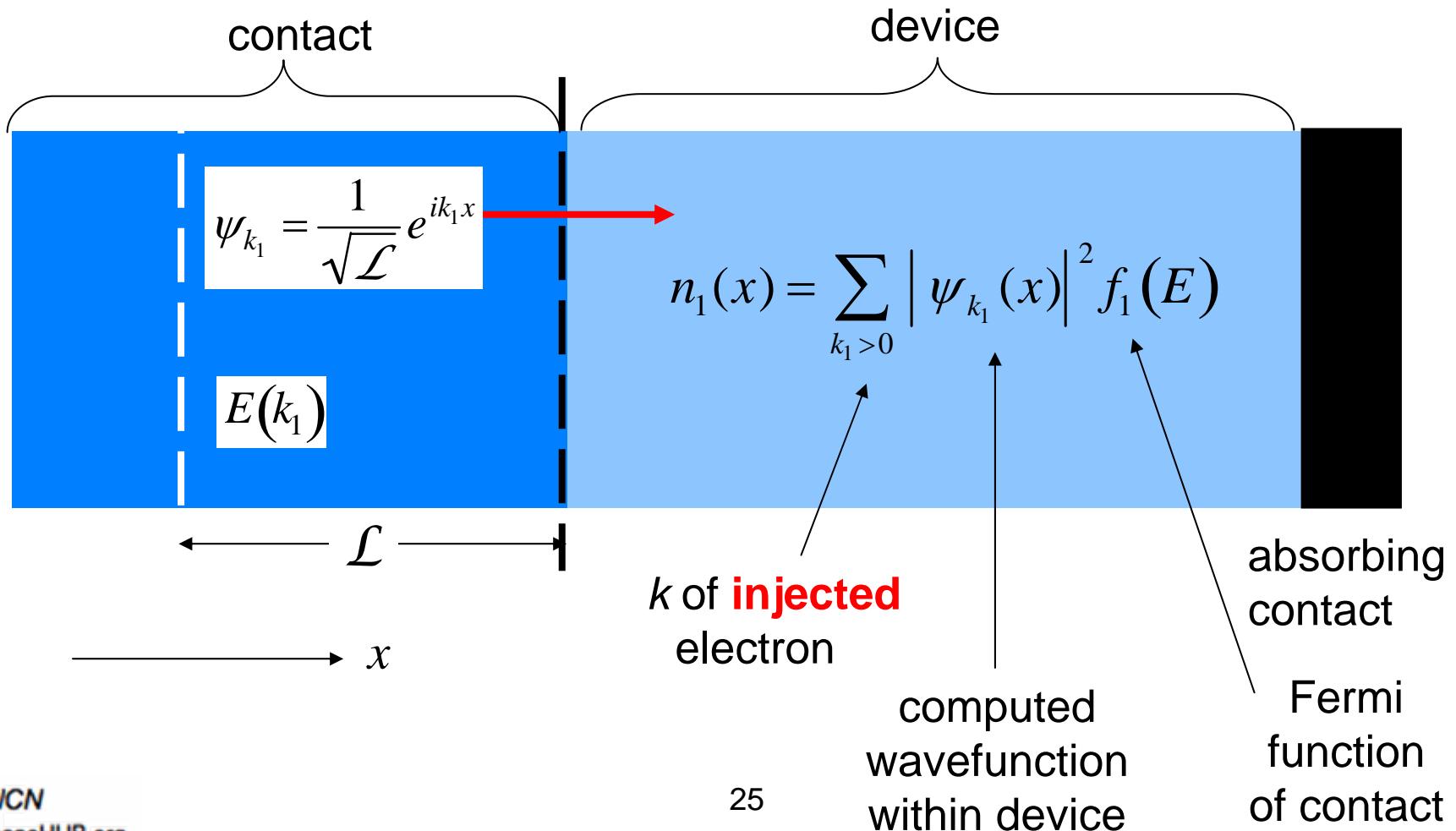
$$\{\psi\} = [G]\{S\}$$

$$[G(E)] = (E[I] - [H] - [\Sigma_1] - [\Sigma_2])^{-1}$$

( $N \times N$  Green's function)

# finding $n(x)$ from $\psi(x)$

*the device is attached to a bulk contact .....*



# finding $n(x)$ from $\psi(x)$

$$n_1(x_i) = \frac{1}{\mathcal{L}} \sum_{k_1 > 0} |\psi_{k_1}(x_i)|^2 f_1(E)$$

$$n_1(x_i) = \int_0^\infty \left[ \frac{1}{\pi} \frac{dk_1}{dE} |\psi_{k_1}(x_i)|^2 \right] f_1(E) dE = \int_0^\infty LDOS(x_i, E) f_1(E) dE$$

Recall:  $g_{1D}(E) = \frac{2}{\pi} \frac{dk_1}{dE}$

Semi-classically:

$$n_1(x_i) = \int_0^\infty \left[ \frac{1}{\pi \hbar} \sqrt{\frac{2m^*}{E - E_C(x_i)}} \right] F_n(x) dE$$

## filling states from two contacts

---

$$n(x_i, E) = LDOS_1(x_i, E)f_1(E) + LDOS_2(x_i, E)f_2(E)$$

$$n(x_i) = \int_0^{\infty} n(x_i, E) dE$$

The LDOS can be computed either semi-classically or quantum mechanically.

# pause and recap

---

1) Solve for the wavefunction as a function of injection energy,  $E$

$$\{\psi\} = [G]\{S\}$$

$$[G(E)] = (E[I] - [H] - [\Sigma_1] - [\Sigma_2])^{-1}$$

2) Compute the local density of states fillable by each contact:

$$[A_{1,2}] = G \Gamma_{1,2} G^+ \quad (\text{spectral function})$$

$$\Gamma_{1,2}(E) = i \left[ \Sigma_{1,2}(E) - \Sigma_{1,2}^+(E) \right] \quad (\text{broadening})$$

$$LDOS_{1,2}(x, E) = 2 \times \frac{1}{2\pi} \text{diag}[A_{1,2}(E)]$$

## pause and recap (ii)

---

3) Fill states:

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

(electron correlation function)

4) Integrate over energy:

$$\rho = 2 \times \frac{1}{2\pi} \int G^n(E) dE \quad (\text{density matrix})$$

$$n(x) = \text{diag}[\rho]$$

But, how do we compute the current?

# current from transmission

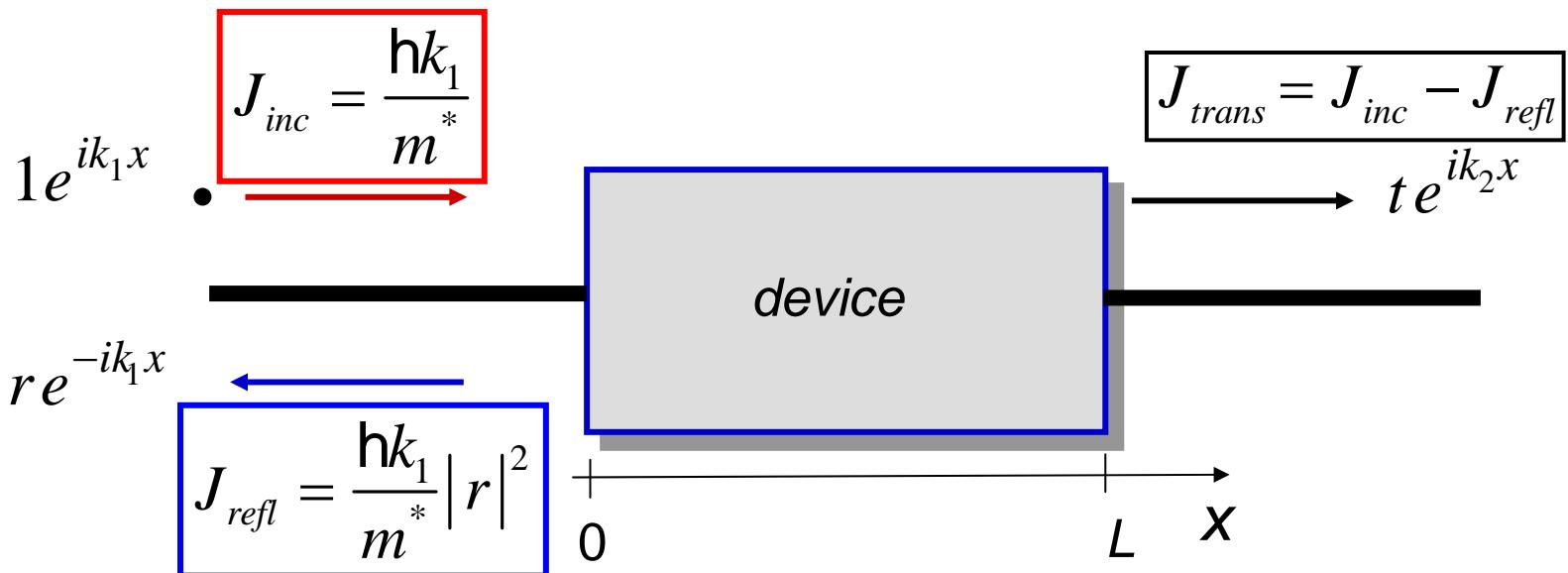
---

$$I(E) = \frac{2q}{h} T(E) M(E) (f_1 - f_2)$$

$$I_D = \int I(E) dE$$

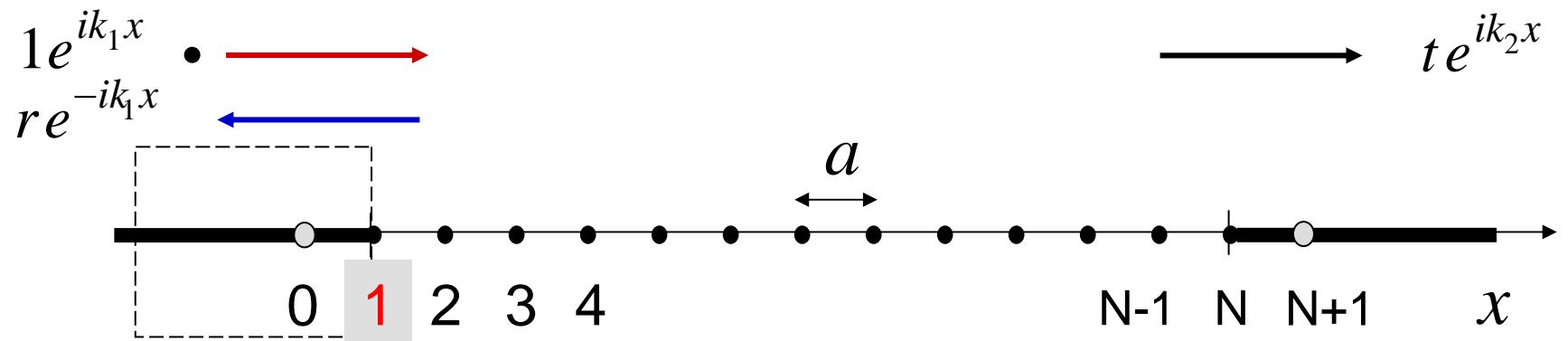
Now, how do we compute the transmission?

# transmission (coherent transport)



$$T_{1-2}(E) = T(E) = \frac{J_{trans}}{J_{inc}} = 1 - \frac{J_{refl}}{J_{inc}} = 1 - |r|^2$$

# finding $r$



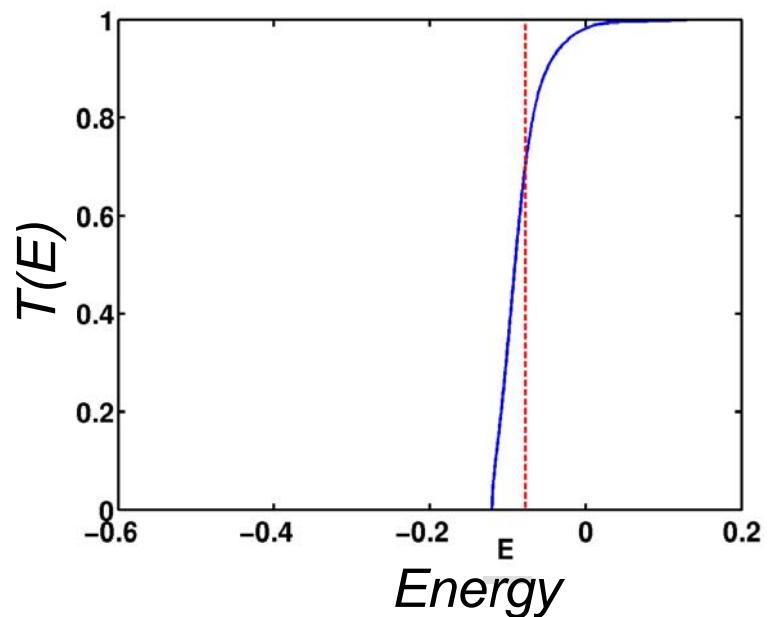
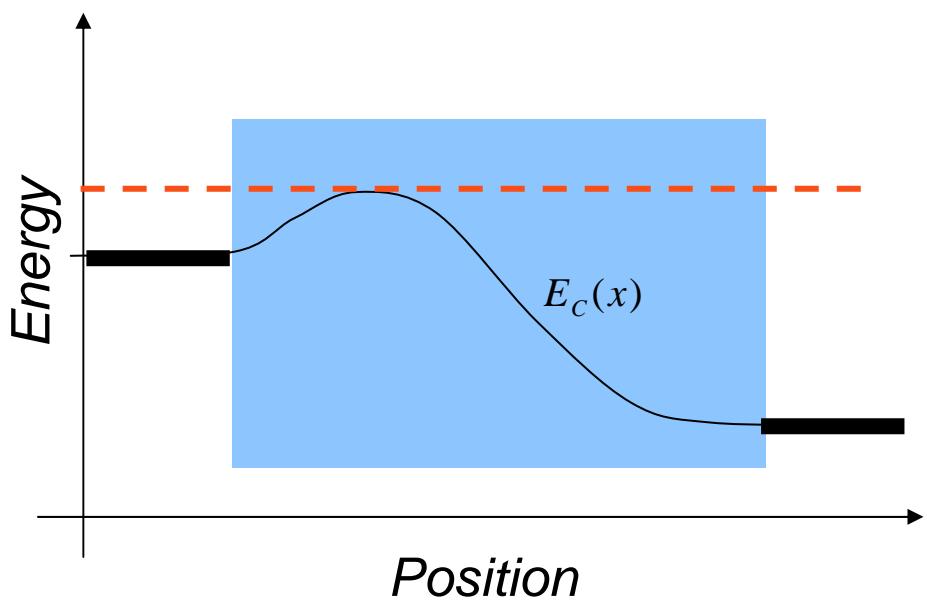
$$\psi(x) = 1e^{ik_1x} + r e^{-ik_1x} \quad x \leq 0$$

$$\psi(x=0) = 1 + r = \psi_1$$

$$T(E) = 1 - |\psi_1 - 1|^2$$

$$T(E) = \text{Trace}\left[\Gamma_1 G \Gamma_2 G^\dagger\right] = \text{Trace}\left[\Gamma_2 G \Gamma_1 G^\dagger\right]$$

# $T(E)$ for a MOSFET



# recap

---

1) Solve for the wave function as a function of injection energy,  $E$

$$\{\psi\} = [G]\{S\}$$

$$[G(E)] = (E[I] - [H] - [\Sigma_1] - [\Sigma_2])^{-1}$$

2) Compute transmission

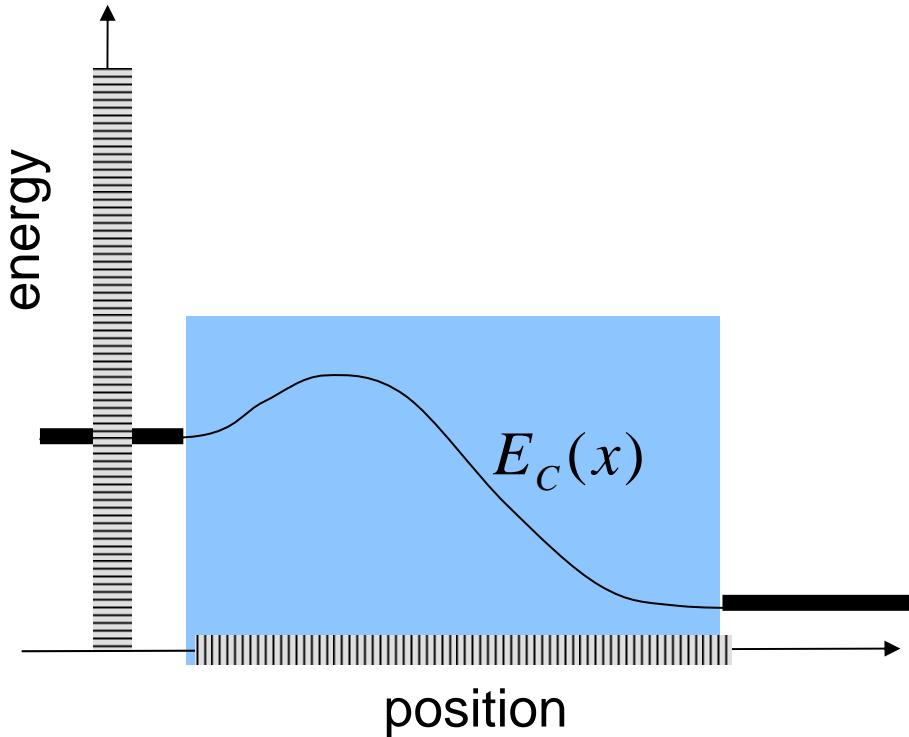
$$T(E) = \text{Trace}[\Gamma_1 G \Gamma_2 G^\dagger] = \text{Trace}[\Gamma_2 G \Gamma_1 G^\dagger]$$

3) Compute current

$$I(E) = T(E)M(E)(f_1 - f_2)$$

$$I_D = \frac{2q}{h} \int_0 I(E) dE$$

# overall simulation procedure (ballistic)



*independent energy channels  
(ballistic)*

- 1) Guess  $E_C(x)$
- 2) For each energy:  
$$(E[I] - [H] - [\Sigma])\{\psi\} = \{S\}$$
- 3) Determine  $n(x)$ :  
$$n(x_i) = n_1(x_i) + n_2(x_i)$$
- 4) solve Poisson for  $E_C(x)$



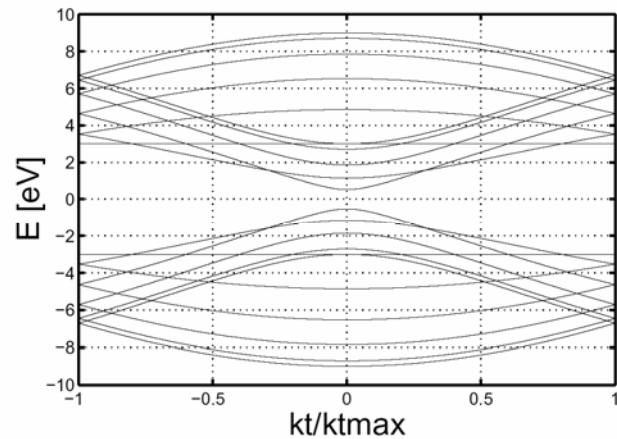
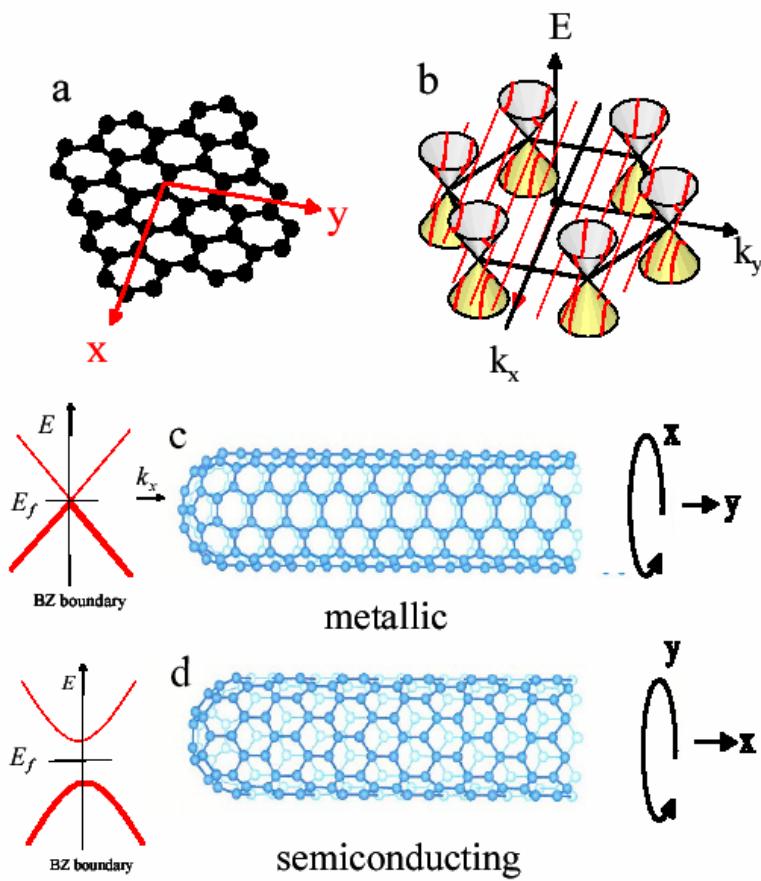
- 5) Determine  $I_D$   
$$I(E) = \frac{2q}{h} \bar{T}(E) (f_1 - f_2)$$
$$I_D = \int I(E) dE$$

# outline

---

- 1) Introduction
- 2) A primer on ballistic quantum transport
- 3) Ballistic quantum transport in CNT MOSFETs**
- 4) A primer on dissipative quantum transport
- 5) Dissipative quantum transport in CNT MOSFETs
- 6) Discussion
- 7) Summary

# carbon nanotubes



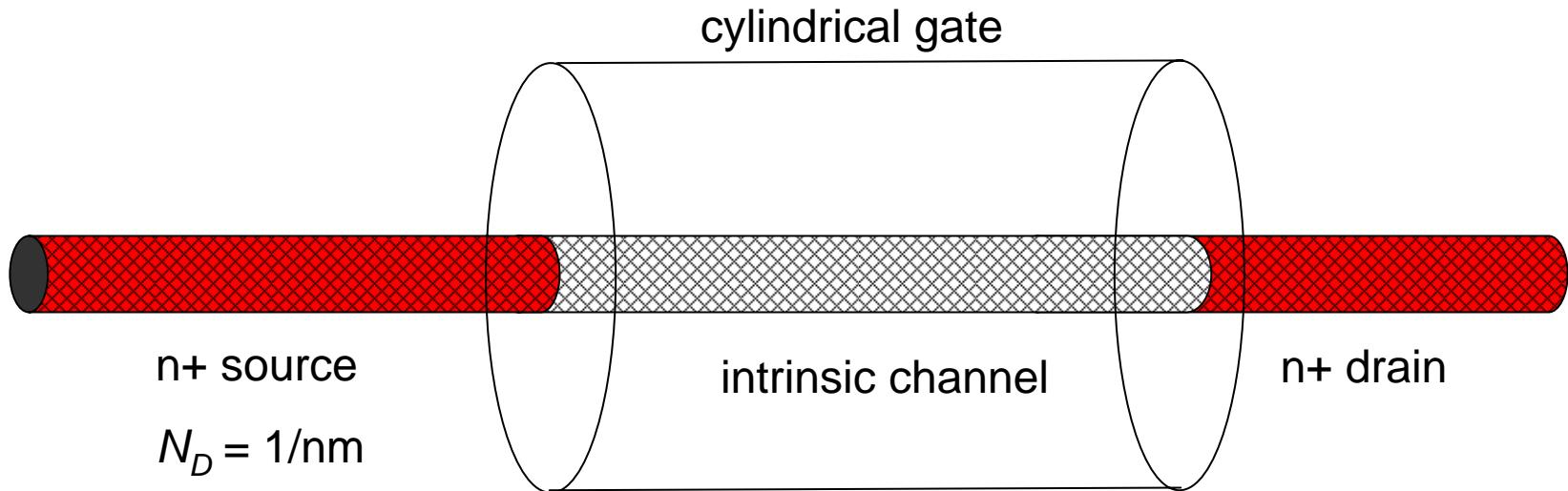
$$E_G \approx 0.8eV/d(\text{nm})$$

$$E(k) = \pm \left( \frac{E_G}{2} \right) \sqrt{1 + (3kd/2)^2}$$

McEuen *et al.*, IEEE Trans. Nanotech., 1 , 78, 2002.

# model device

---



- 1) carbon nanotube, (13, 0),  $D = 1 \text{ nm}$ ,  $E_G = 0.8 \text{ eV}$ )
- 2) gate insulator,  $k = 4$ ,  $t = 4 \text{ nm}$
- 3) channel length,  $L = 12 \text{ nm}$
- 4) power supply,  $V_{DD} = 0.7\text{V}$

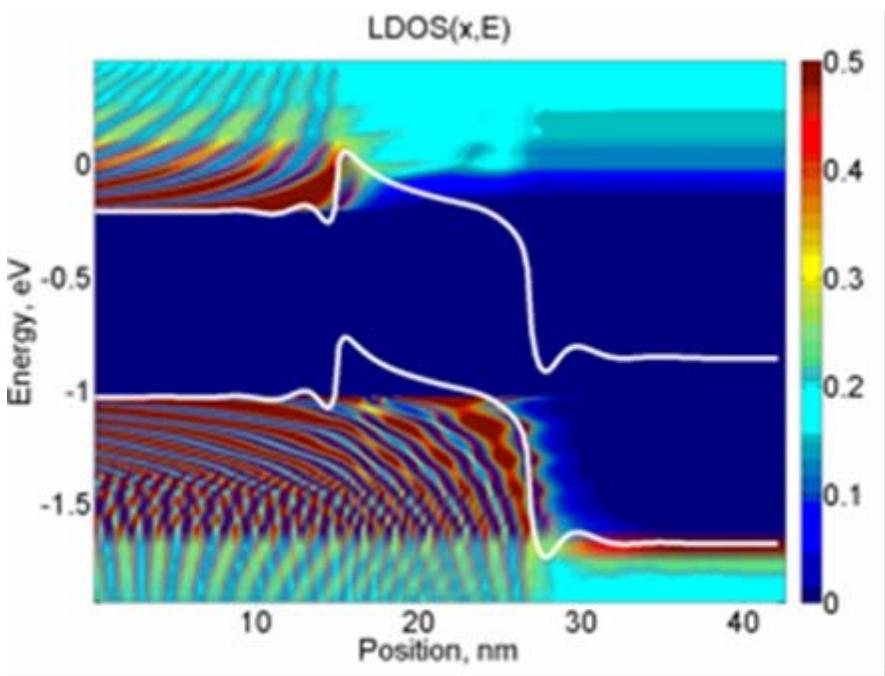
# acknowledgment

---

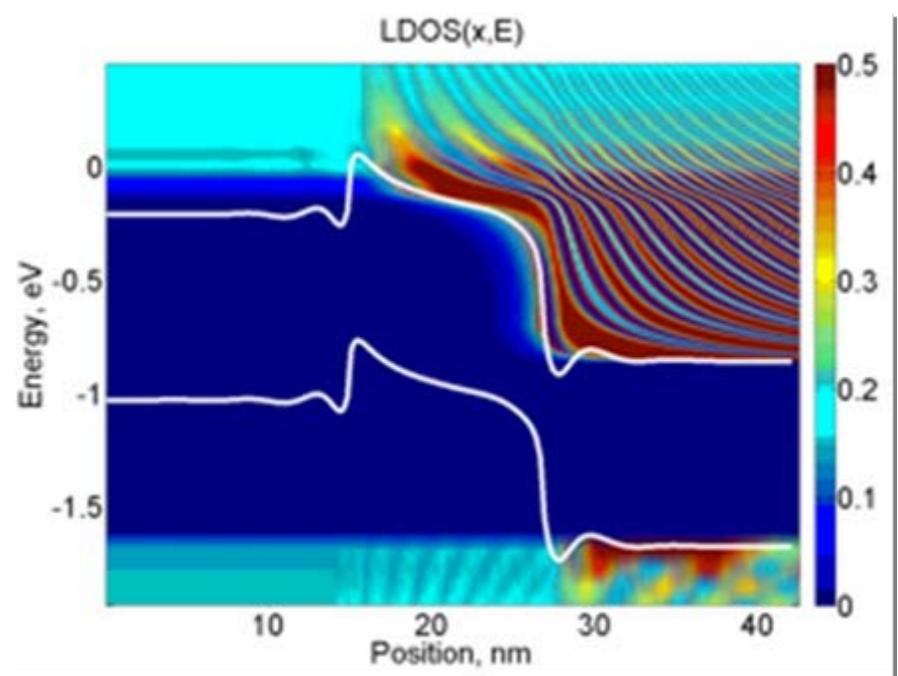
Thanks to Siyu Koswatta (Purdue), and Dmitri Nikonov (Intel), who developed the NEGF simulation code for CNT MOSFETs

and to Yunfei Gao and Gloria Budiman (Purdue) who performed the simulations.

# LDOS(1, 2) at $V_{GS} = V_{DS} = 0.7V$

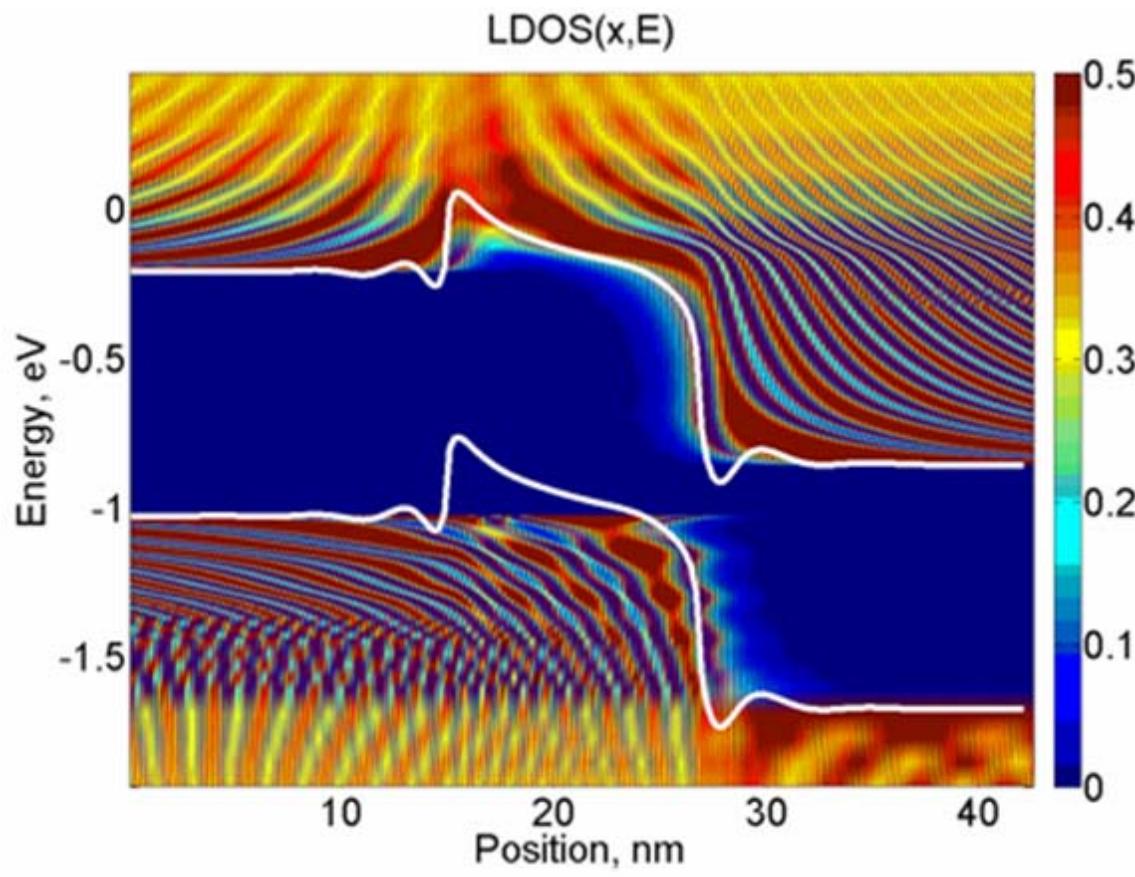


source-injected



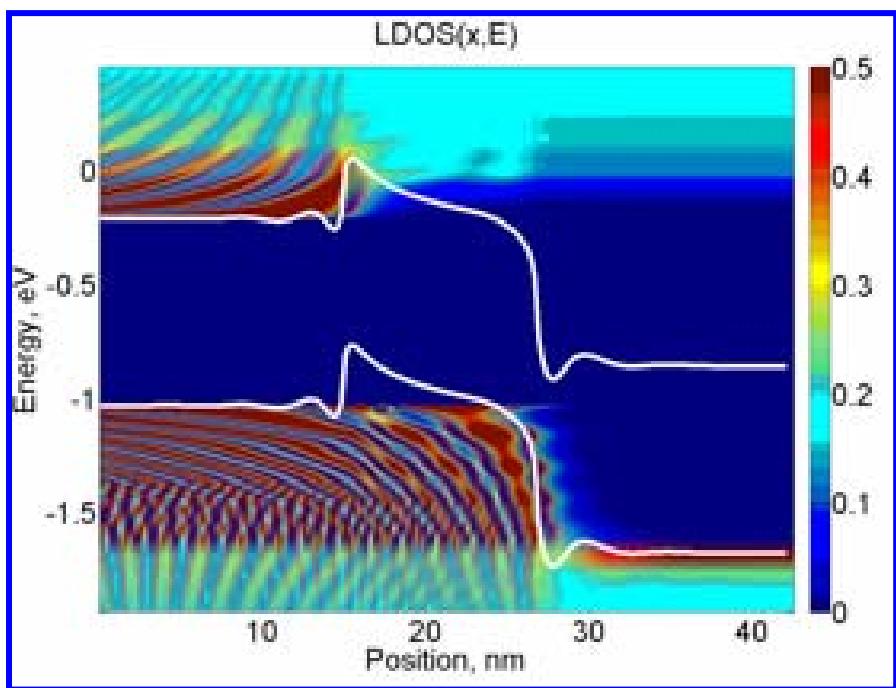
drain-injected

# LDOS(total) at $V_{GS} = V_{DS} = 0.7V$

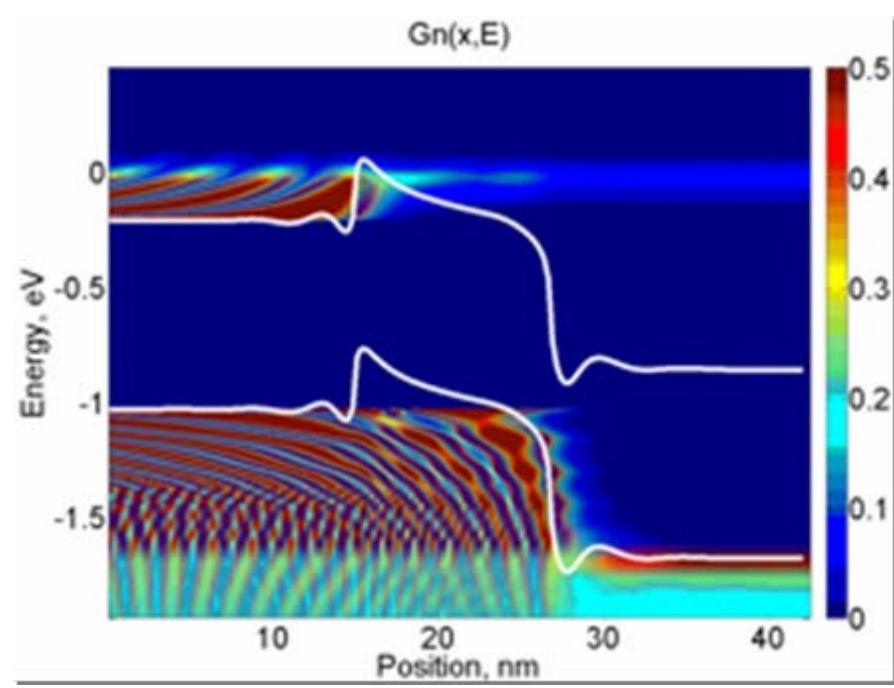


source + drain-injected

$n_1(x, E)$  at  $V_{GS} = V_{DS} = 0.7V$

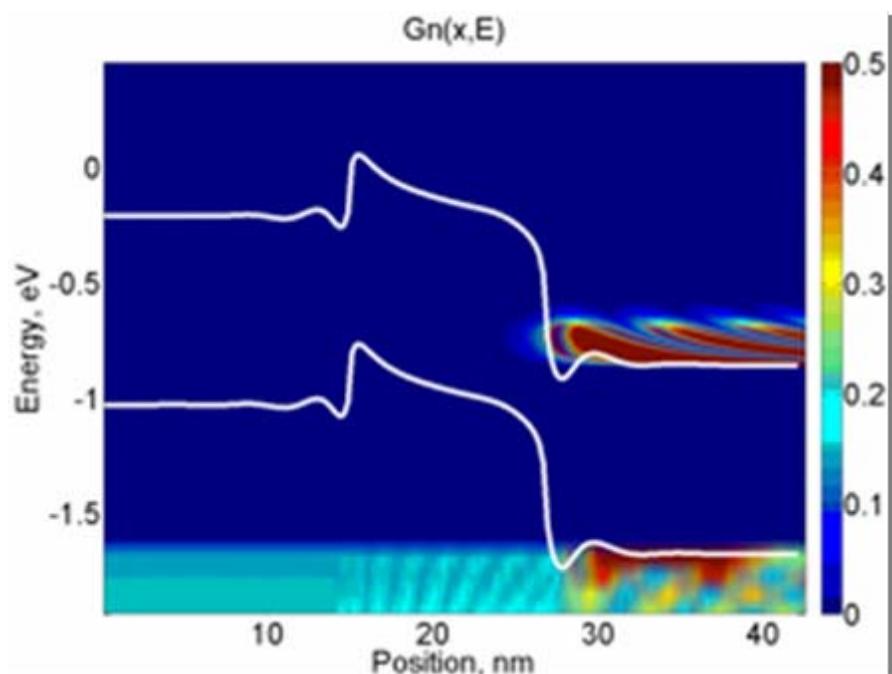
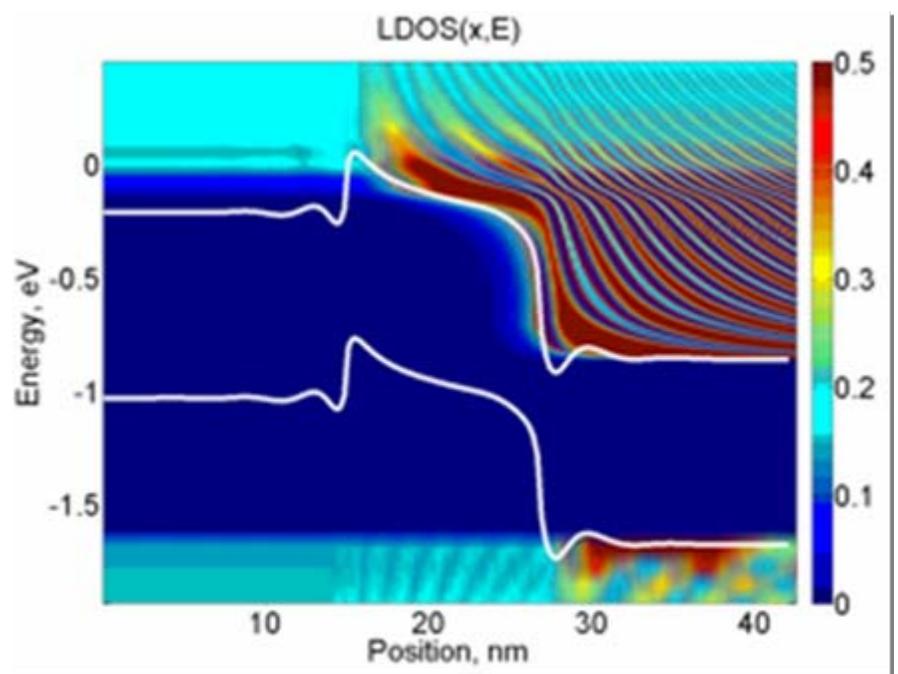


$\text{LDOS}_1(x, E)$



$n_1(x, E)$

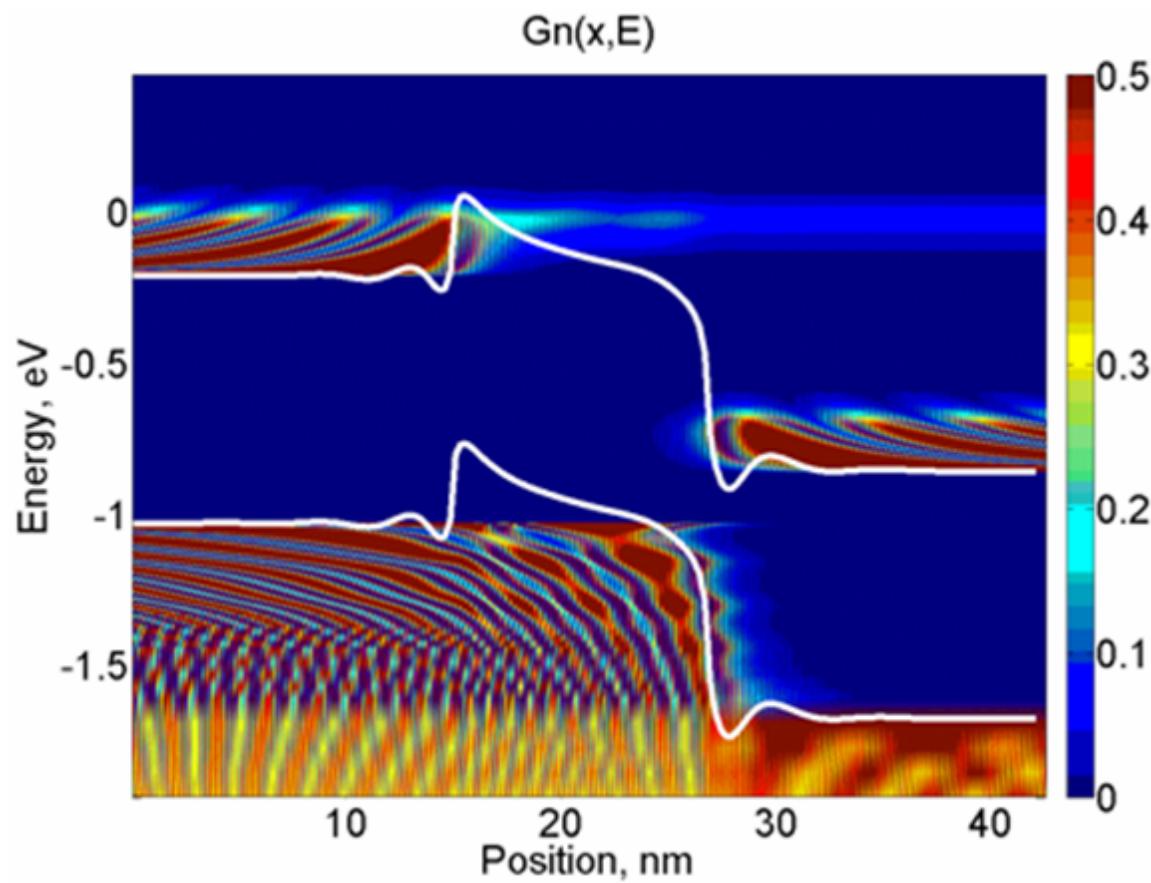
$n_2(x, E)$  at  $V_{GS} = V_{DS} = 0.7V$



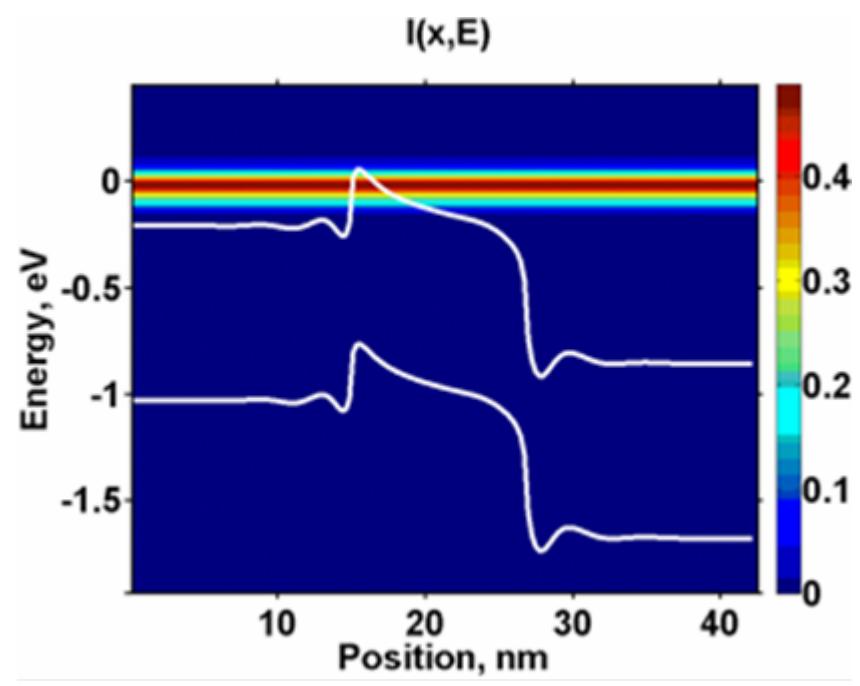
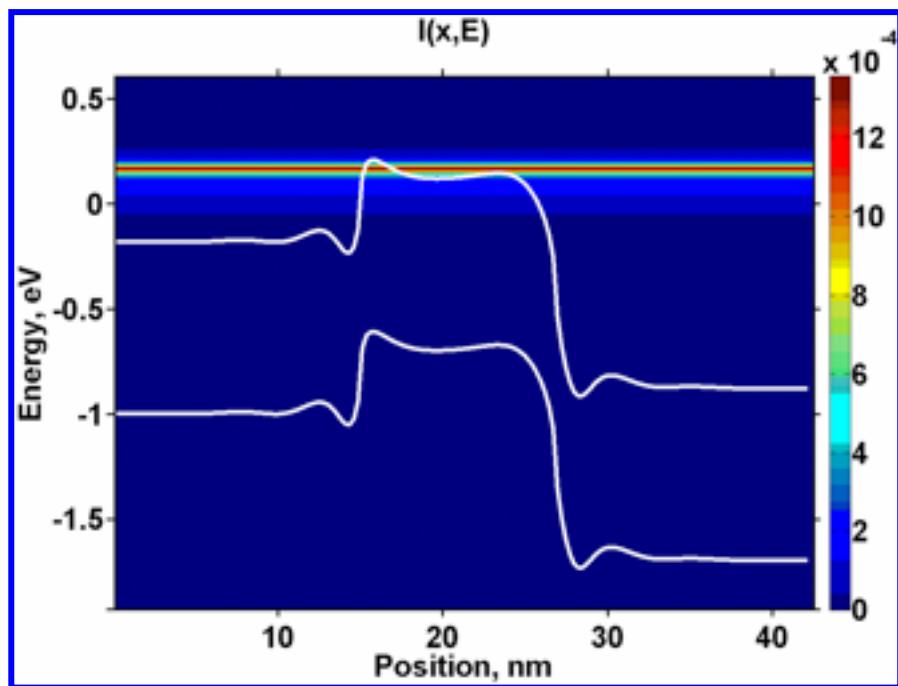
$\text{LDOS}_2(x, E)$

$n_2(x, E)$

$n_{TOT}(x, E)$  at  $V_{GS} = V_{DS} = 0.7V$



$I(x, E)$  at  $V_{DS} = 0.7V$



$V_{GS} = 0.0V$

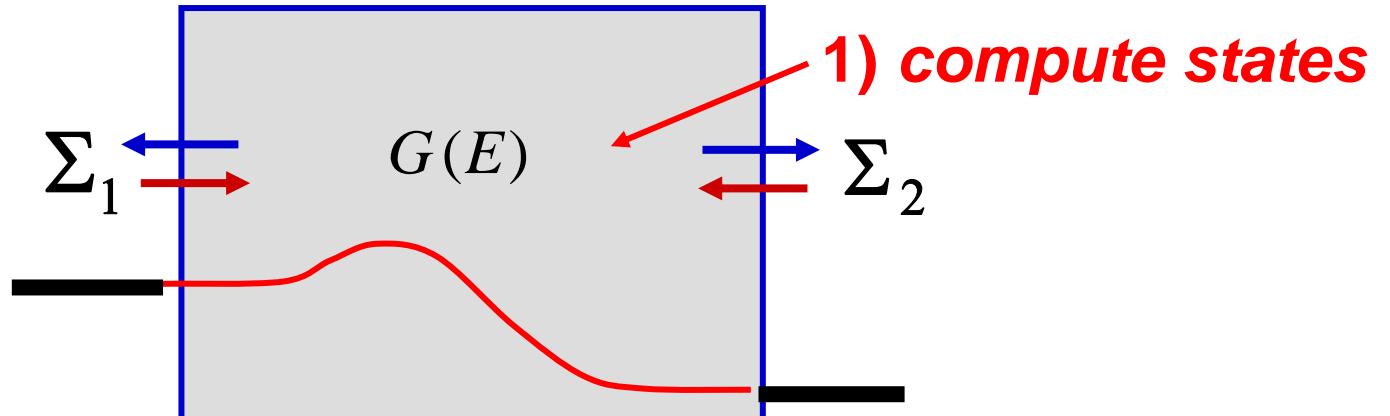
$V_{GS} = 0.7V$

# outline

---

- 1) Introduction
- 2) A primer on ballistic quantum transport
- 3) Ballistic quantum transport in CNT MOSFETs
- 4) A primer on dissipative quantum transport**
- 5) Dissipative quantum transport in CNT MOSFETs
- 6) Discussion
- 7) Summary

# review: filling states (ballistic)



1) **compute states**

2) **fill states**

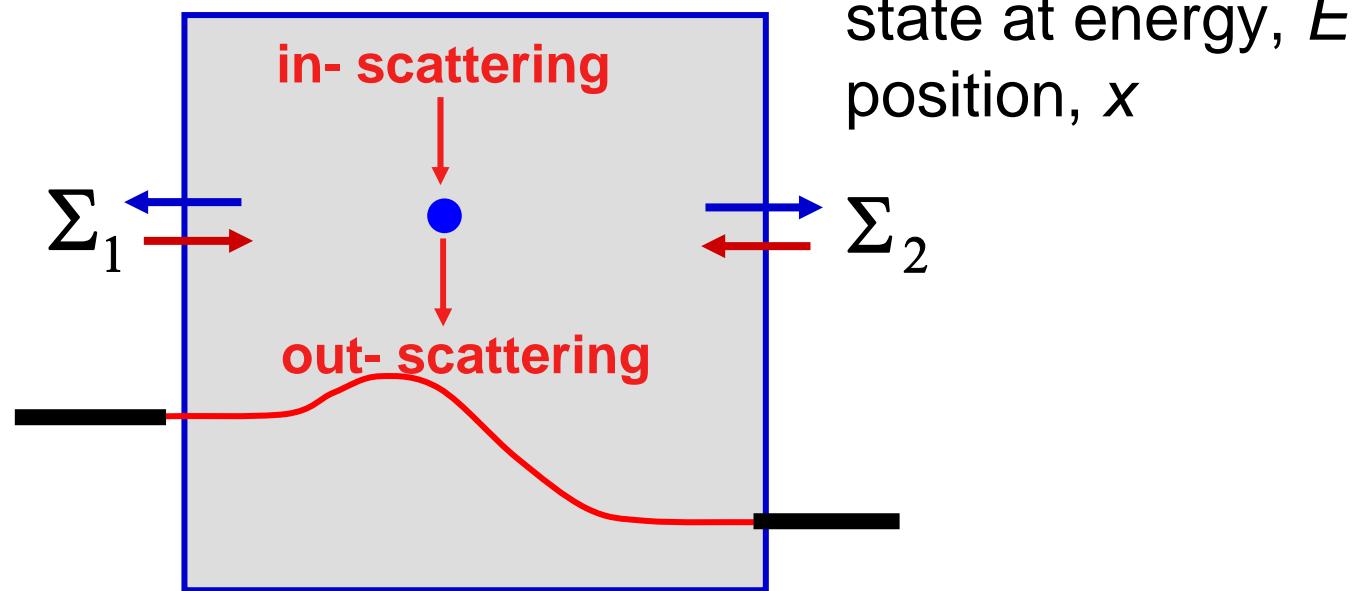
$$[G^n(E)] = [A_1(E)]f_1(E) + [A_2(E)]f_2(E)$$

$$[A_1] = G \Gamma_1 G^\dagger$$

$$[G^n(E)] = G [\Gamma_1 f_1(E)] G^\dagger + G [\Gamma_2 f_2(E)] G^\dagger$$

$$[G^n(E)] = G \Sigma_{in} G^\dagger \quad [\Sigma^{in}] = [\Gamma_1] f_1 + [\Gamma_2] f_2$$

# filling states through scattering



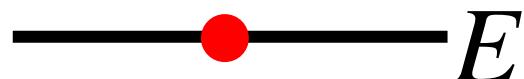
$$[G(E)] = [E[I] - [H] - [\Sigma_1] - [\Sigma_2] - [\Sigma_S]]^{-1}$$

$$[G^n(E)] = G \left( \Sigma_1^{in} + \Sigma_2^{in} + \Sigma_S^{in} \right) G^+$$

# example: dissipative (phonon) scattering

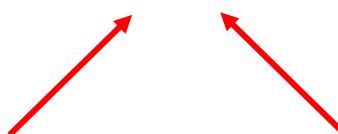
---

'in-scattering'  
from contact 1



$$[G^n(E)] = [G] [\Sigma_1^{in}] [G^+]$$

$$[\Sigma_1^{in}] = [\Gamma_1] f_1$$

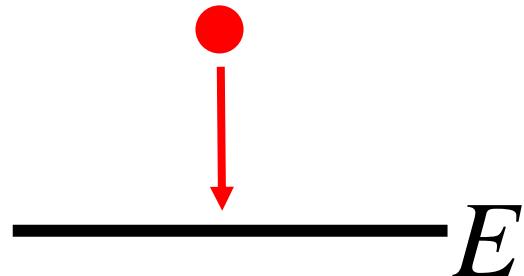


strength of connection  
to source

population  
of source

## phonon scattering (ii)

in-scattering  
from another state



$$[G^n(E)] = [G] [\Sigma_S^{in}] [G^+]$$

$$[\Sigma_S^{in}] \sim [D] [G_n]$$

strength of connection  
to phonons

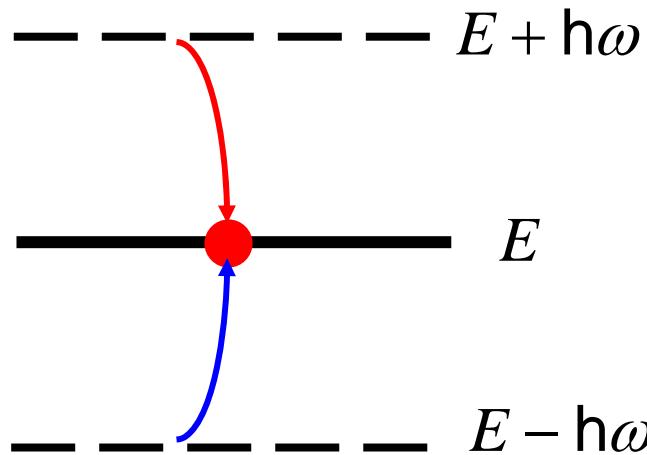
(unknown) population  
of source



## phonon scattering (iii)

# *phonon emission*

# *phonon absorption*



$$\Sigma_S^{in}(E) \approx D_0(N_\omega + 1)G^n(E + \hbar\omega) + D_0N_\omega G^n(E - \hbar\omega)$$

**(emission)**                                   **(absorption)**

Notice:  $\left[ \Sigma_S^{in} \right]$  depends on  $\left[ G^n \right]$

# out-scattering

---

Recall that for ballistic transport:

$$[G^n(E)] = G\Sigma^{in}G^\dagger \quad [\Sigma^{in}] = [\Gamma_1]f_1 + [\Gamma_2]f_2$$

There is also an ‘out-scattering’ function:

$$[G^p(E)] = G\Sigma^{out}G^\dagger \quad [\Sigma^{out}] = [\Gamma_1](1-f_1) + [\Gamma_2](1-f_2)$$

Note that:

$$[\Sigma^{in}] + [\Sigma^{out}] = [\Gamma] \quad [\Gamma_{1,2}] = i([\Sigma_{1,2} - \Sigma_{1,2}^\dagger])$$

# self-energy for phonon scattering

$$\left[ \Sigma_s^{in} \right] + \left[ \Sigma_s^{out} \right] = \left[ \Gamma_s \right] \quad \left[ \Gamma_s \right] = i \left( \left[ \Sigma_s - \Sigma_s^\dagger \right] \right)$$

Given  $\left[ \Sigma_s^{in} \right]$  and  $\left[ \Sigma_s^{out} \right]$ , what is  $\left[ \Sigma_s \right]$  ?

$$\left[ \Sigma_s(E) \right] = \frac{1}{2} \int \frac{\Gamma_s(E')}{E' - E} dE' - \frac{i\Gamma_s(E)}{2}$$

Frequently, we ignore the real part of the self-energy and assume:

$$\left[ \Sigma_s(E) \right]; -\frac{i\Gamma_s(E)}{2}$$

# solution procedure

1) Solve:

$$[G(E)] = [E[I] - [H] - [\Sigma_1] - [\Sigma_2] - [\Sigma_S]]^{-1}$$

*solve by iteration!*

2) Compute:

$$\begin{aligned}[G^n(E)] &= [G][\Sigma_1^{in}][G]^\dagger + [G][\Sigma_2^{in}][G]^\dagger \\ &\quad + [G][\Sigma_S^{in}][G]^\dagger\end{aligned}$$

*depends on  $[G^n]$*

3) Solve Poisson's equation

# scattering and the density-of-states

---

similar to ballistic case

$$[A(E)] = [G] [\Gamma_1] [G]^\dagger + [G] [\Gamma_2] [G]^\dagger$$

$$+ [G] [\Gamma_s] [G]^\dagger$$



phonon-induced states

# computing current with dissipative scattering

---

$$I(E) \neq T(E)M(E)(f_1 - f_2)$$

$$I_i(E) = \text{Trace}\left(\left[\Sigma_{in}^i\right][A]\right) - \text{Trace}\left(\left[\Gamma_S\right][G^n]\right)$$

# quantum transport with scattering

---

1) Add an appropriate self-energy to the Green's function

$$[G(E)] = (E[I] - [H] - [\Sigma_1] - [\Sigma_2] - [\Sigma_S])^{-1}$$

2) Fill states from contacts and by scattering

$$[G^n(E)] = [G][\Sigma_1^{in}][G]^\dagger + [G][\Sigma_2^{in}][G]^\dagger + [G][\Sigma_S^{in}][G]^\dagger$$

3) Iterate to compute  $[G]$  and again for  $E_C(x)$

4) Compute current

$$I_i(E) = \text{Trace}([\Sigma_{in}^i][A]) - \text{Trace}([\Gamma_s][G^n])$$

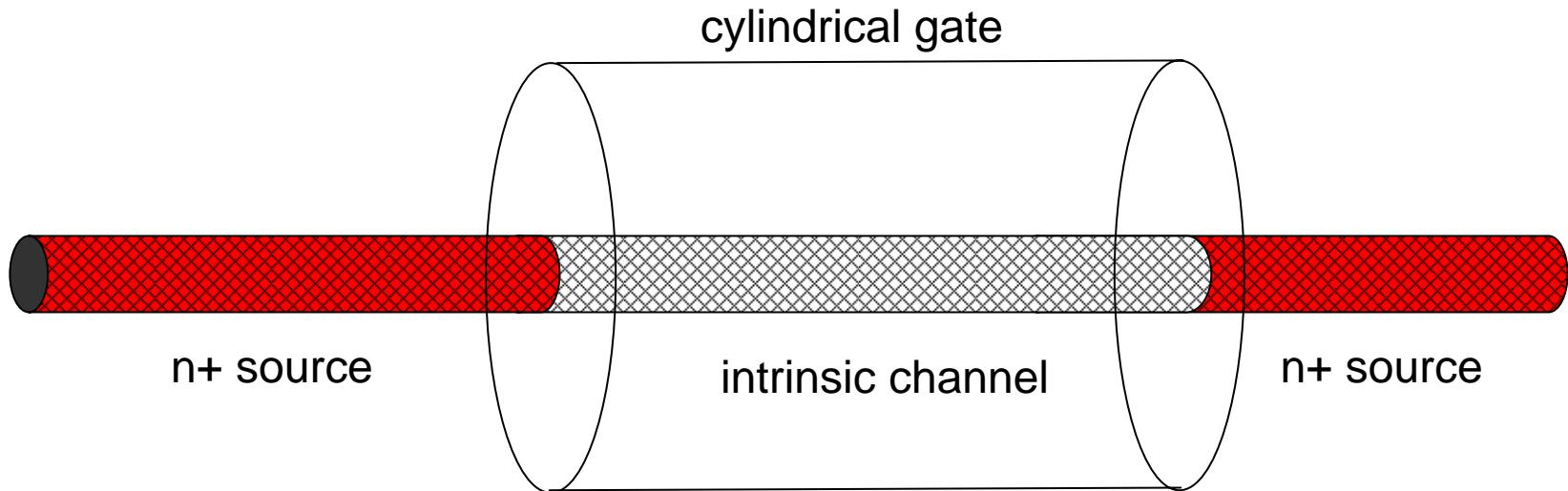
# outline

---

- 1) Introduction
- 2) A primer on ballistic quantum transport
- 3) Ballistic quantum transport in CNT MOSFETs
- 4) A primer on dissipative quantum transport
- 5) Dissipative quantum transport in CNT MOSFETs**
- 6) Discussion
- 7) Summary

# model device

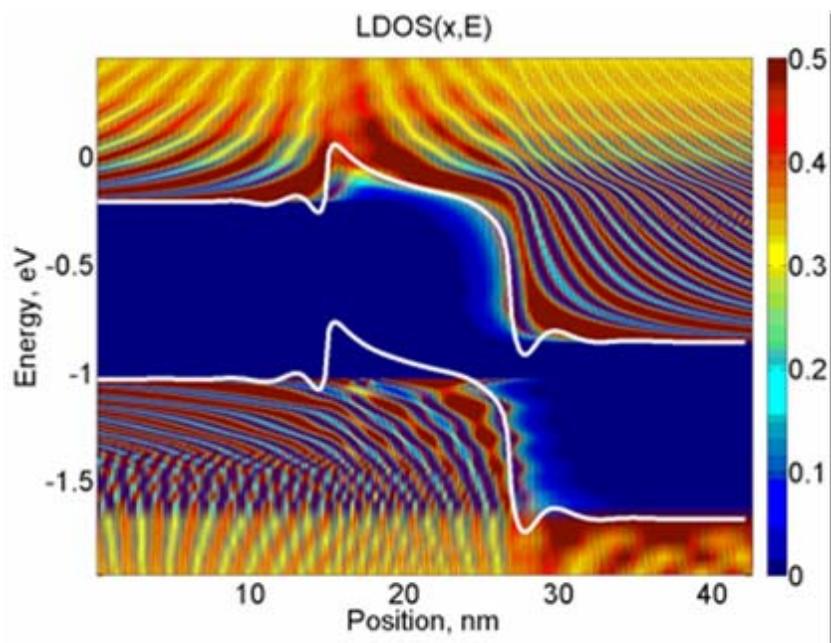
---



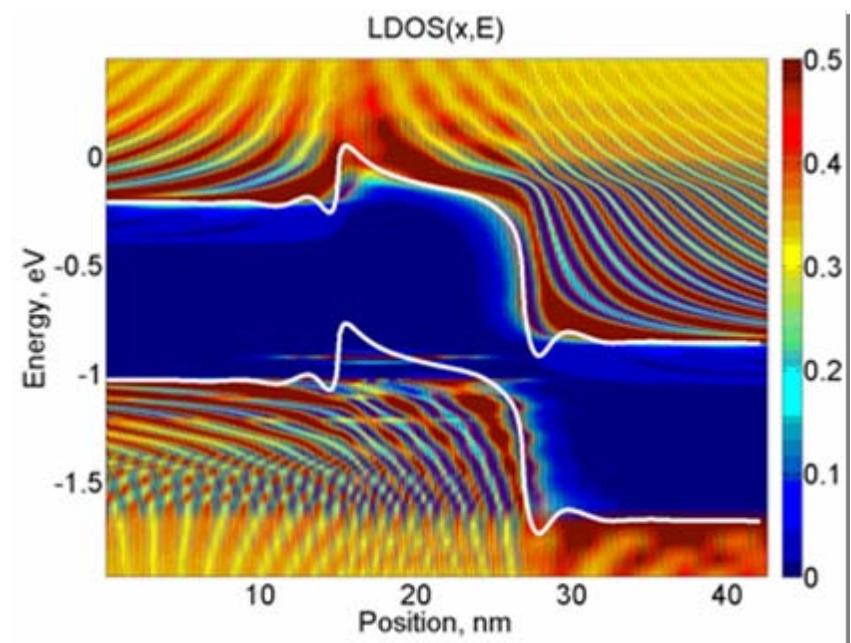
- 1) acoustic phonons
- 2) optical (zone center and zone boundary) phonons

Siyuranga O. Koswatta, Sayed Hasan, and Mark S. Lundstrom, M. P. Anantram, Dmitri E. Nikonov, “Non-equilibrium Green's function treatment of phonon scattering in carbon nanotube transistors,” *IEEE Trans. Electron Dev.*, **54**, 2339, 2007.

# LDOS at $V_{GS} = V_{DS} = 0.7$ V

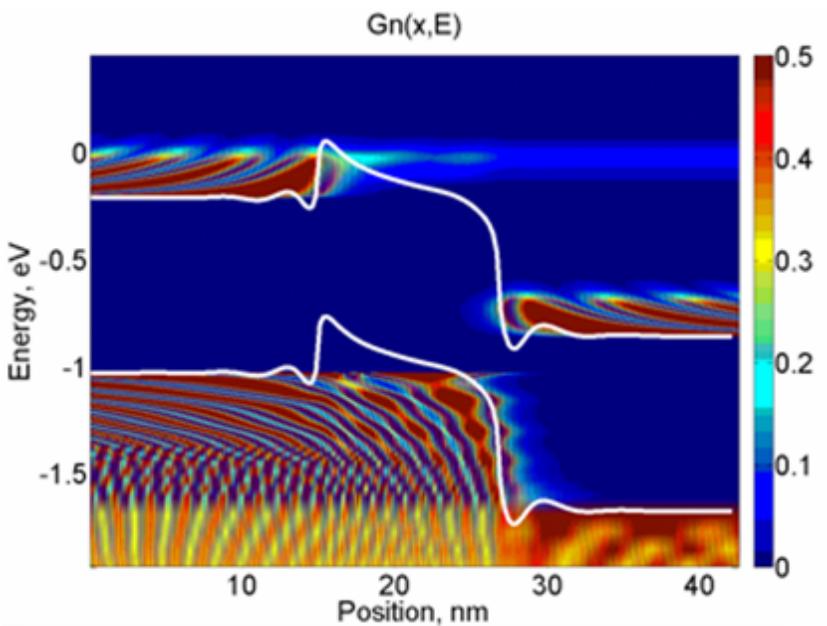


ballistic

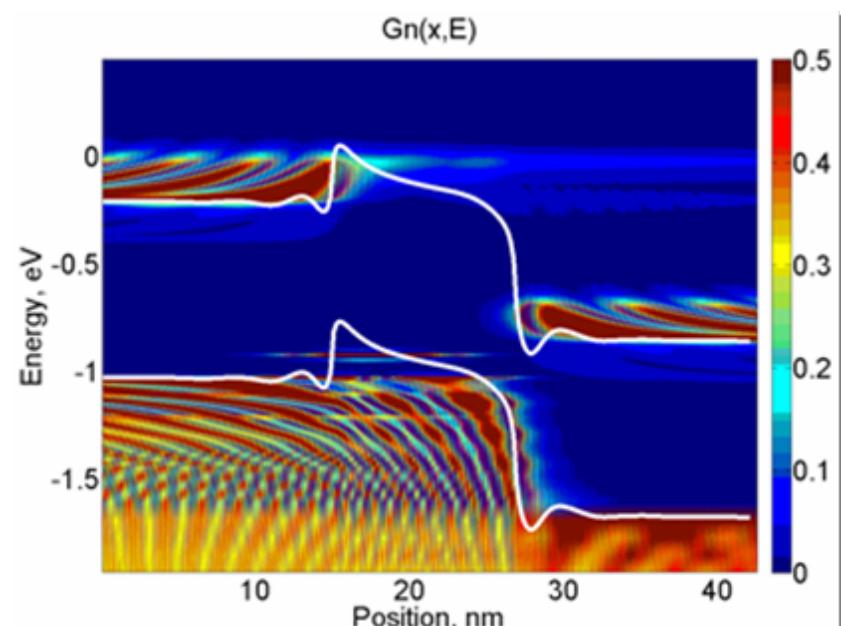


dissipative

$$n(x, E) \text{ at } V_{GS} = V_{DS} = 0.7 \text{ V}$$

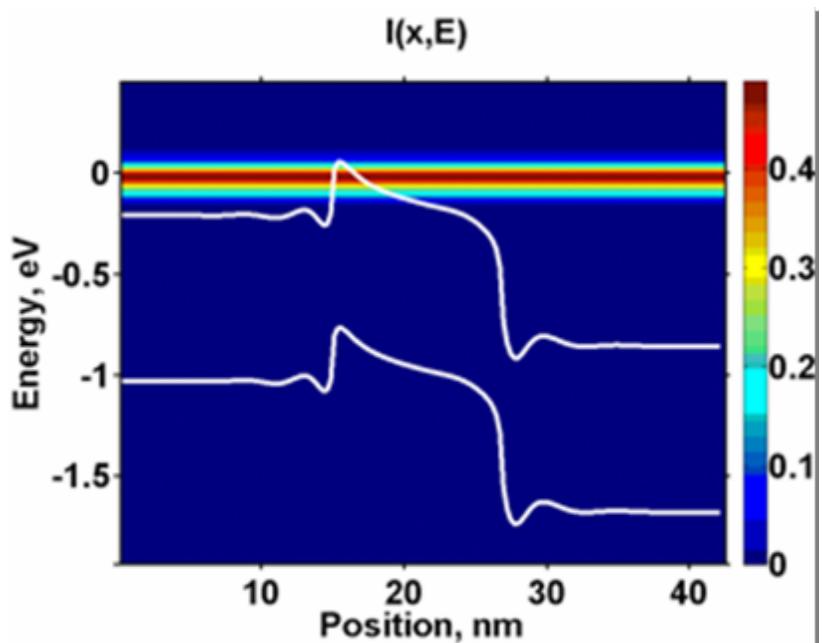


ballistic

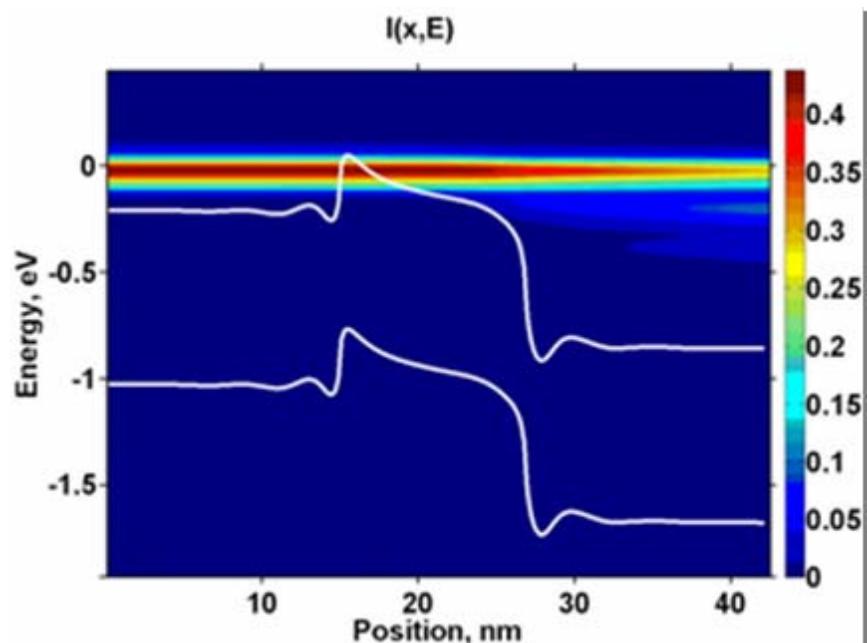


dissipative

$I(x, E)$  at  $V_{GS} = V_{DS} = 0.7$  V

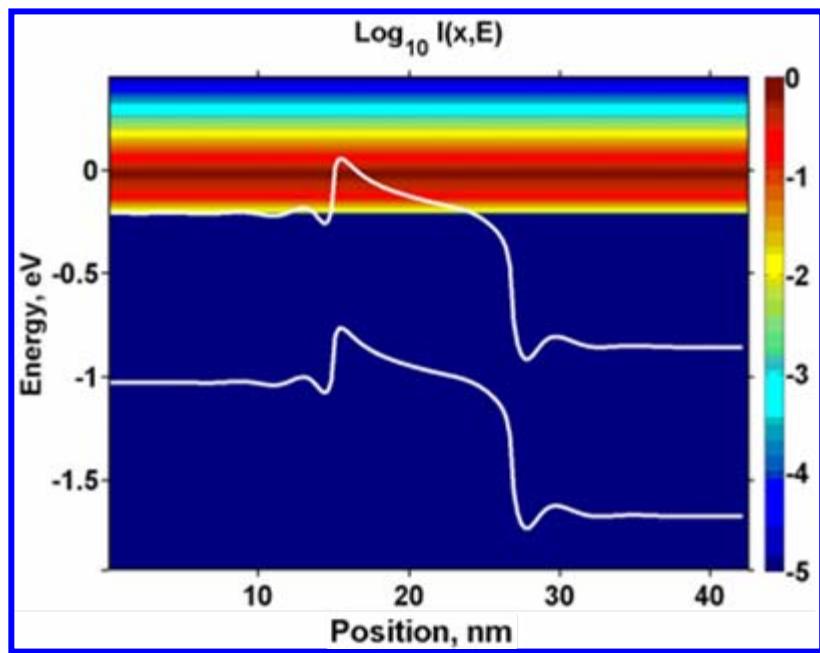


ballistic

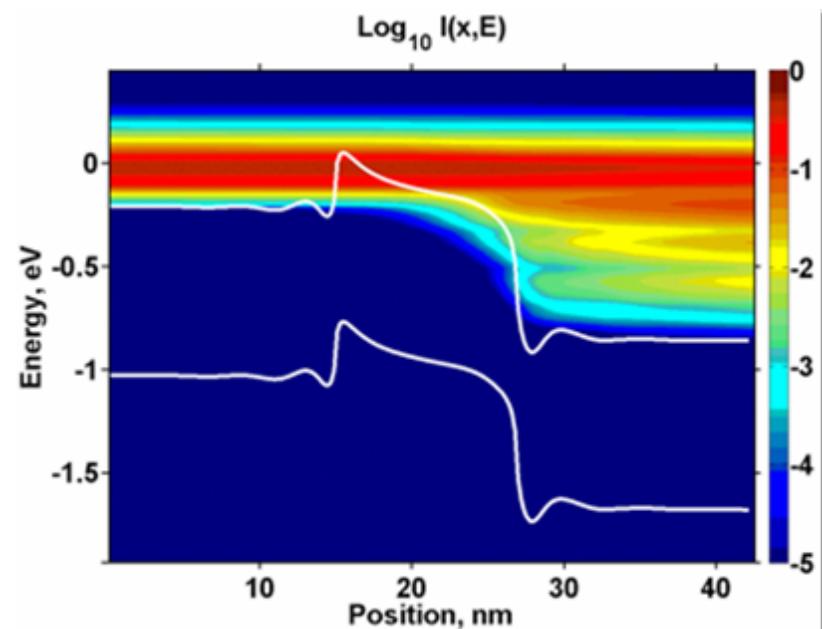


dissipative

$\log I(x, E)$  at  $V_{GS} = V_{DS} = 0.7$  V



ballistic



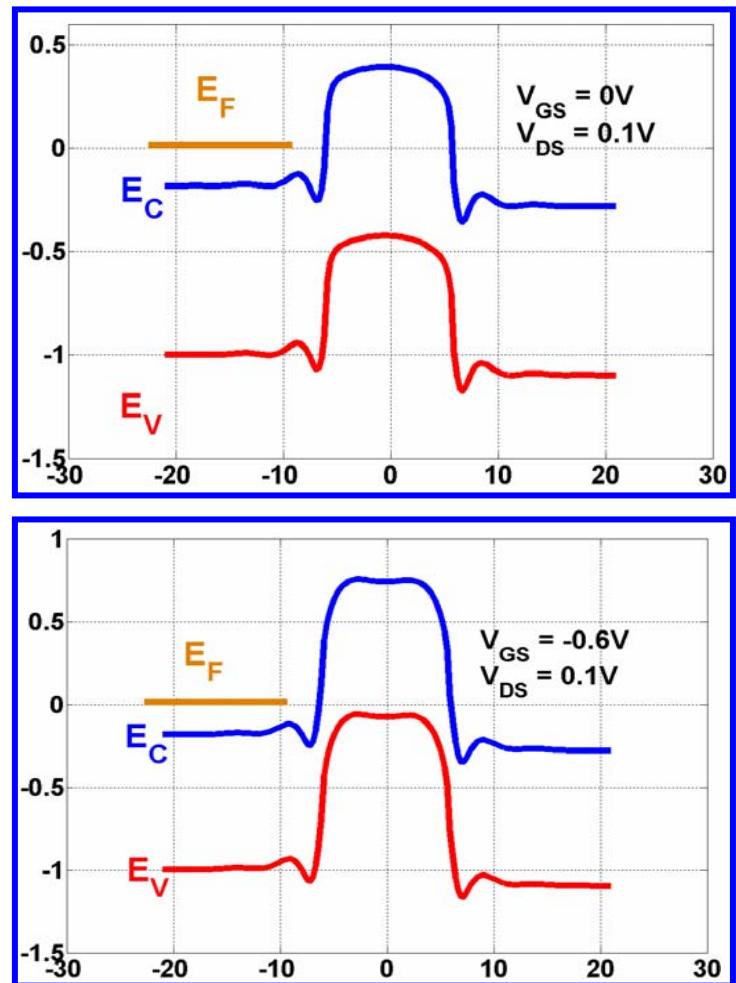
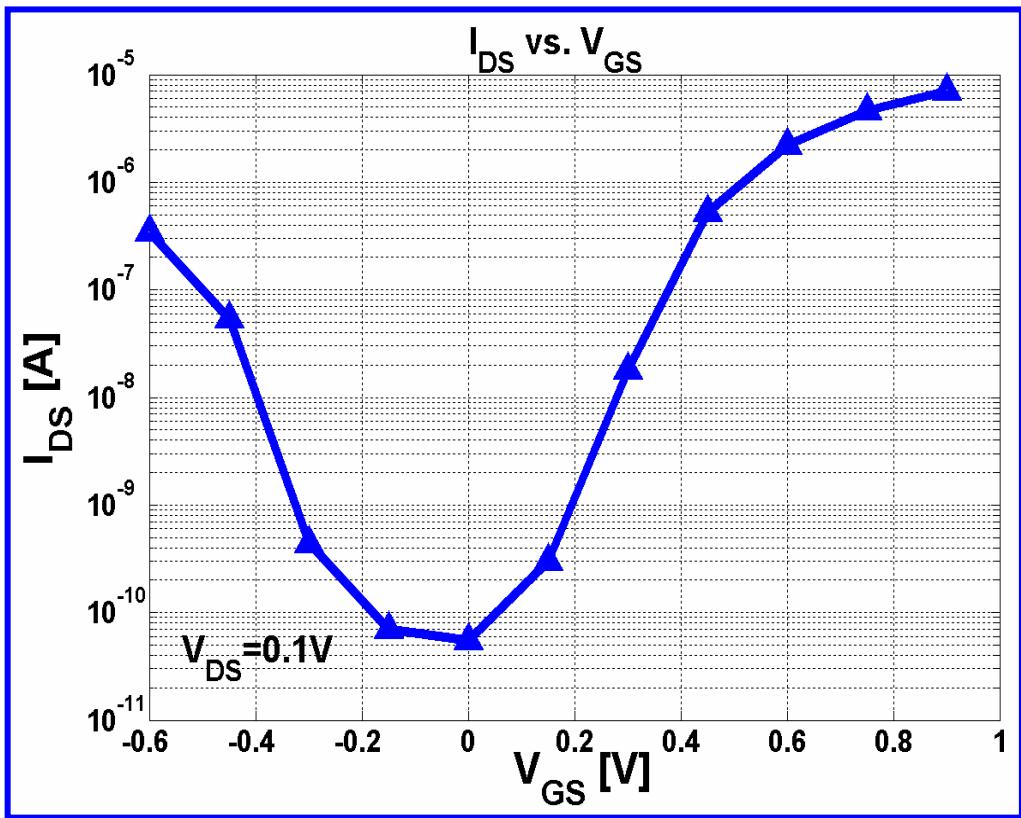
dissipative

# outline

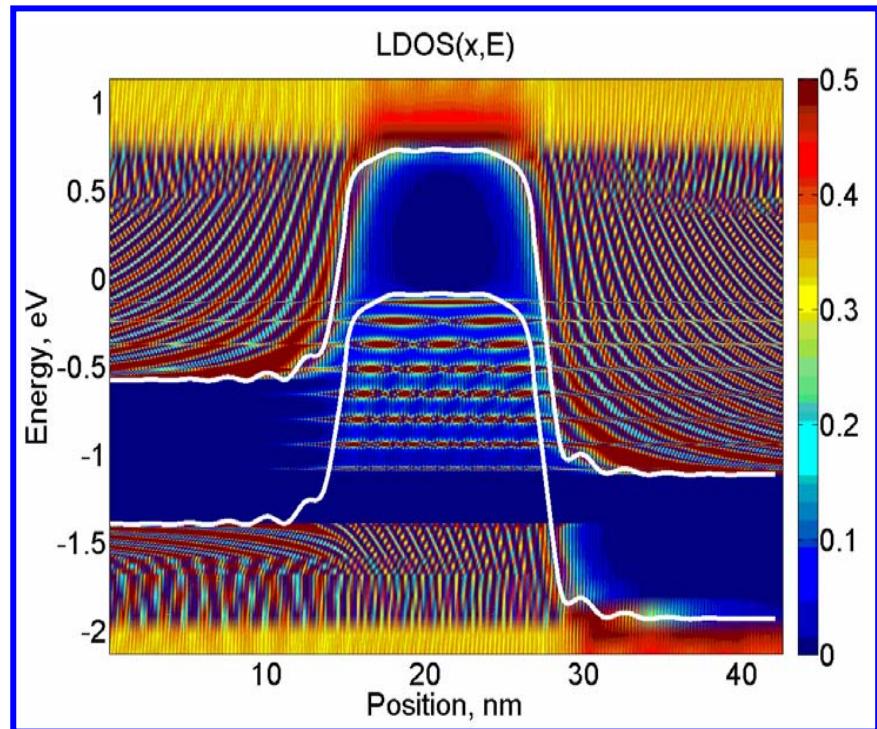
---

- 1) Introduction
- 2) A primer on ballistic quantum transport
- 3) Ballistic quantum transport in CNT MOSFETs
- 4) A primer on ballistic quantum transport
- 5) Dissipative quantum transport in CNT MOSFETs
- 6) Discussion**
- 7) Summary

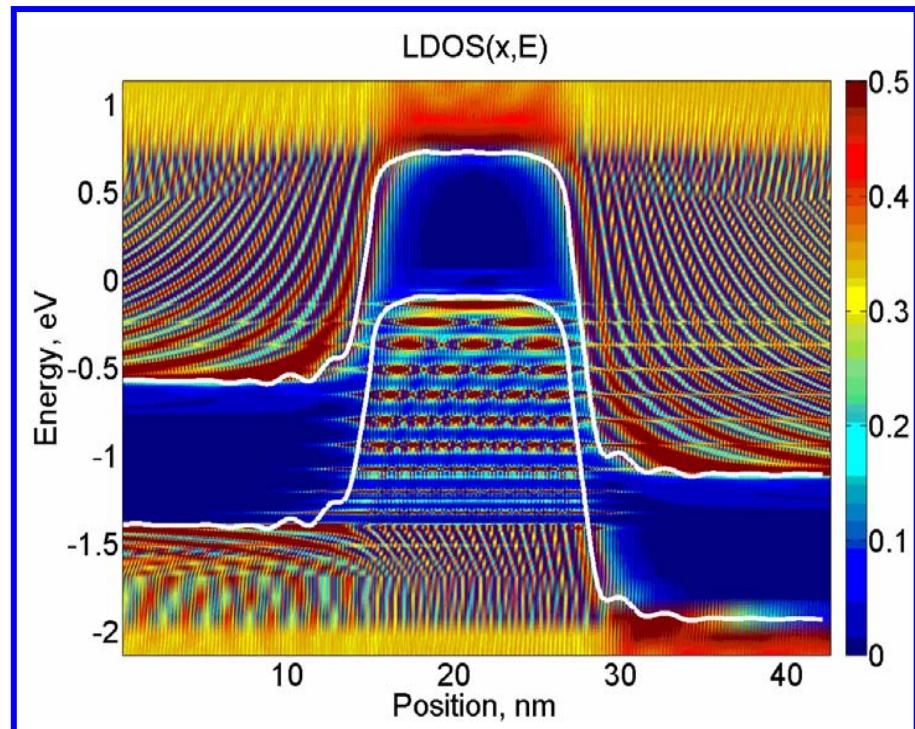
# *band-to-band tunneling*



# LDOS at $V_{GS} = -0.6V$ $V_{DS} = 0.6 V$

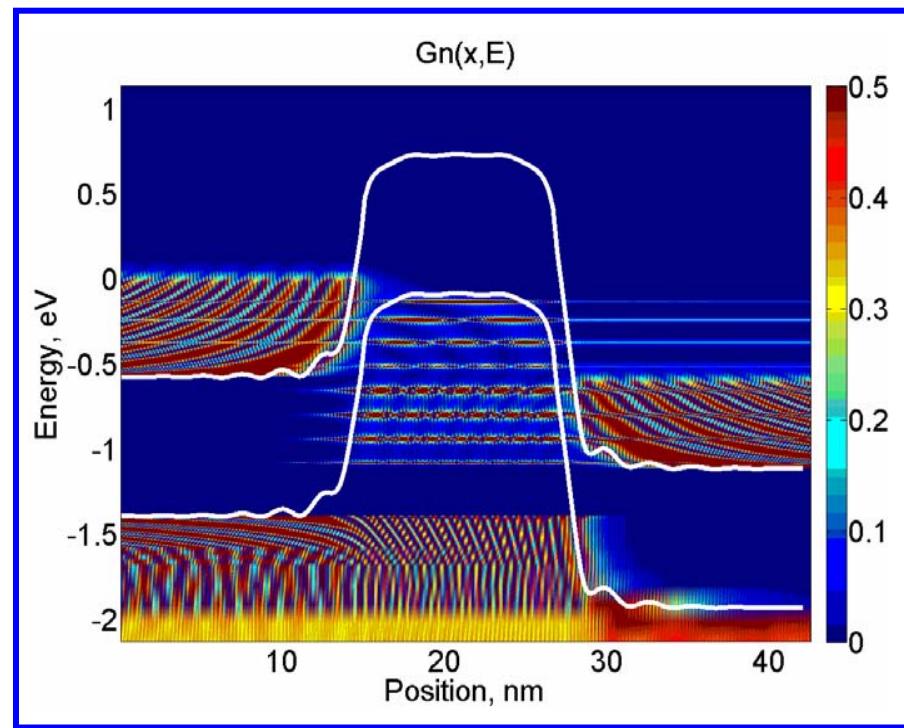


ballistic

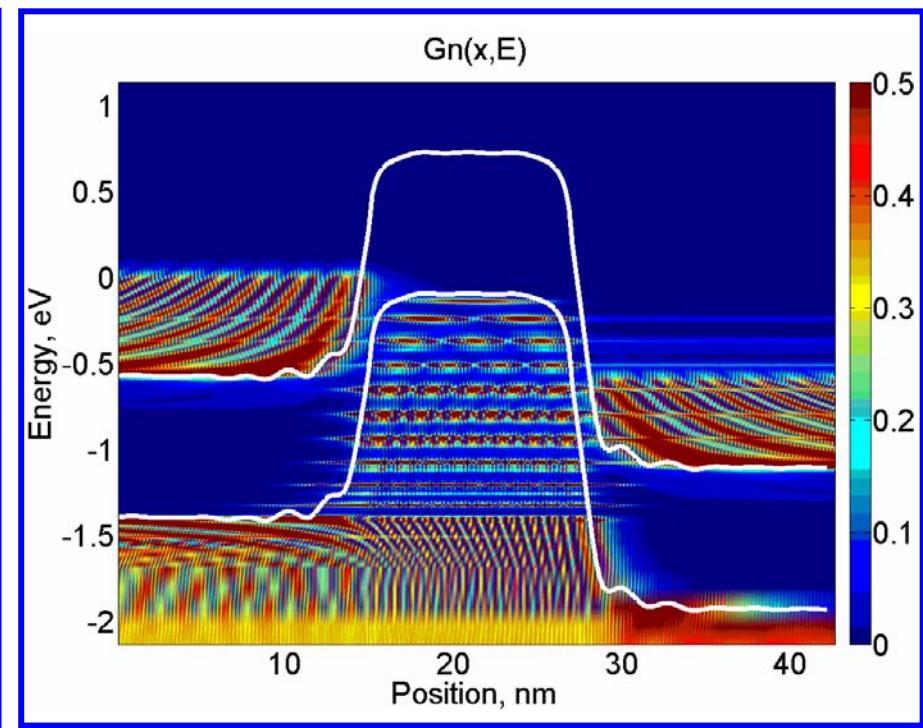


dissipative

$n(x, E)$  at  $V_{GS} = -0.6V$   $V_{DS} = 0.6 V$

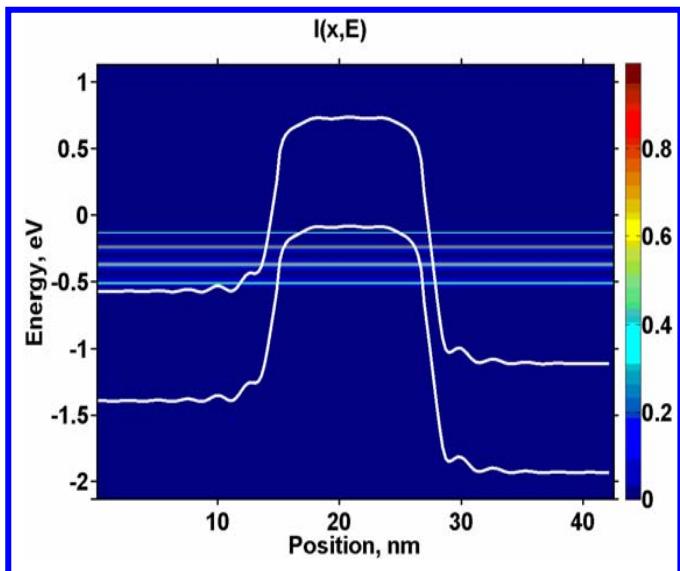


ballistic

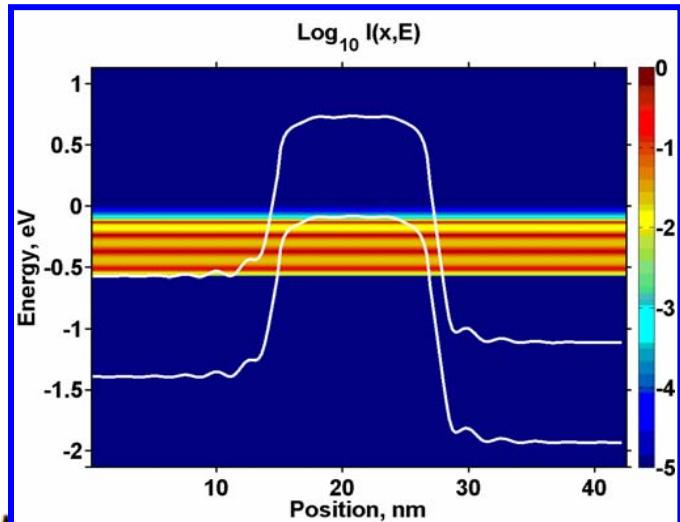
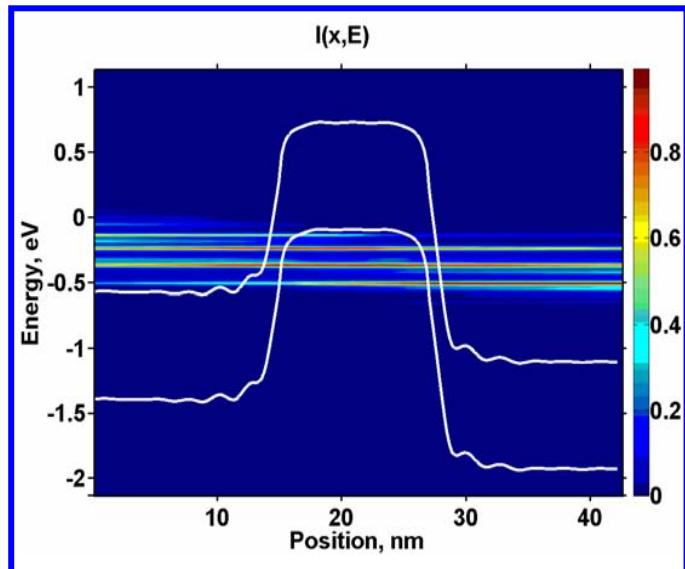


dissipative

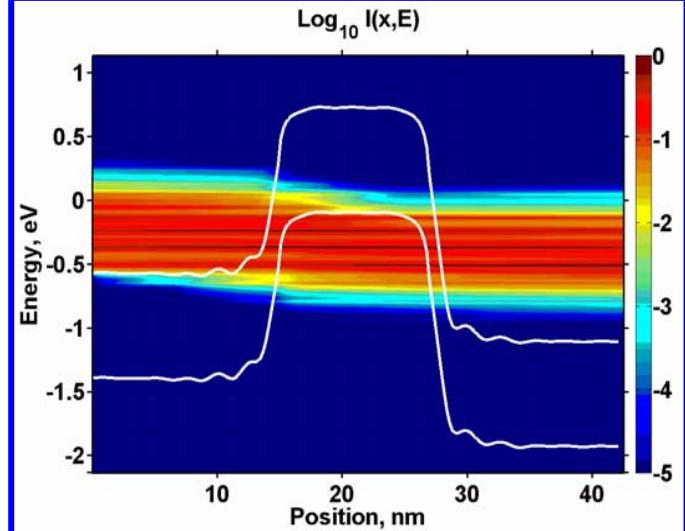
$$I(x, E) \text{ at } V_{GS} = -0.6V \ V_{DS} = 0.6V$$



linear



log



ballistic

dissipative

# quantum vs. semi-classical transport

---

## 1) Boltzmann Transport Equation

$f(r, k)$  In equilibrium, this is the Fermi function.  
6D, 3 in position and 3 in momentum space

## 2) Non-equilibrium Green's function formalism

$[G(r, r', E)]$  7D because  $E$  is an independent variable.

Energy channels are coupled for dissipative scattering.

# outline

---

- 1) Introduction
- 2) A primer on ballistic quantum transport
- 3) Ballistic quantum transport in CNT MOSFETs
- 4) A primer on dissipative quantum transport
- 5) Dissipative quantum transport in CNT MOSFETs
- 6) Discussion
- 7) Summary**

# QM and MOSFETs

---

- 1) *MOSFETs are, by design, remarkably classical devices.*
- 2) *But quantum mechanics does affect very small MOSFETs by:*
  - 1) increasing  $V_T$
  - 2) decreasing  $C_S$  (inv) and, therefore,  $C_G$ (on)
  - 3) affecting transport along the channel
    - intraband tunneling
    - band-to-band tunneling