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SPRING COLLEGE ON SCIENCE AT THE NANOSCALE
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Simulating Quantum Transport in Ballistic Nanowire FETS

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These are preliminary lecture notes, intended only for distribution to participants.

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Simulating Quantum Transport in Ballistic Nanowire FETs

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1) **Introduction**
2) **Solving the Wave Equation**
3) **Computing n(x)**
4) **Computing I_D**
5) **Discussion**
6) **Summary**

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I) Introduction: device simulation

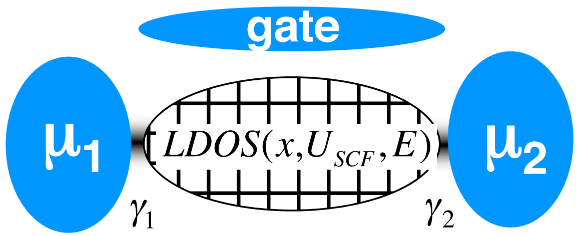
"Poisson" Equation

$$n(\mathbf{r}) \rightarrow E_C(\mathbf{r})$$

Transport Equation

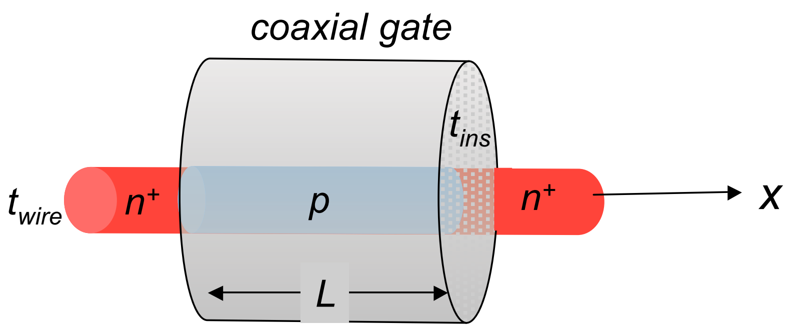
$$E_C(\mathbf{r}) \rightarrow n(\mathbf{r})$$

- Boltzmann Transport Equation
- Schrödinger Equation
- NEGF
- etc.

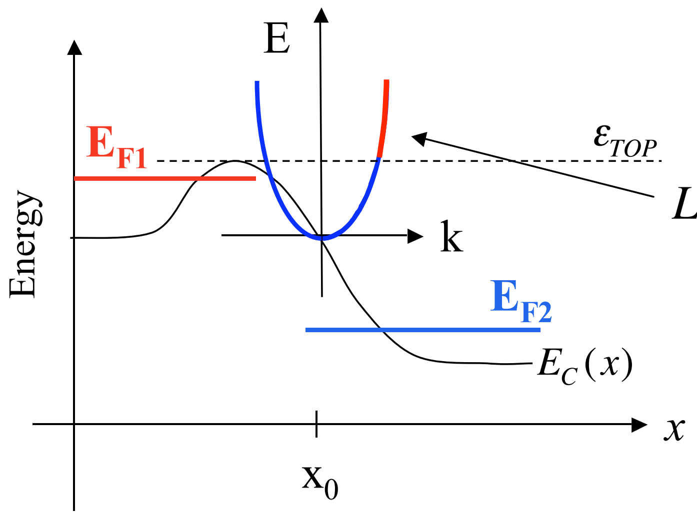


1) Compute U_{SCF}
2) Compute LDOS
   Fill LDOS

I) Introduction: nanowire MOSFET

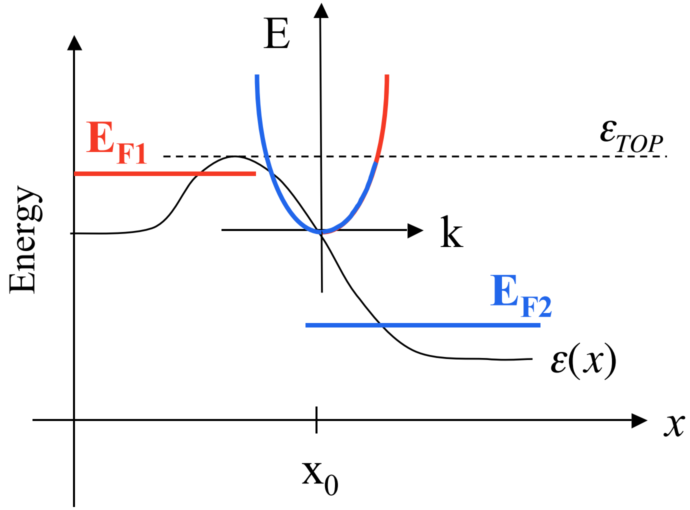


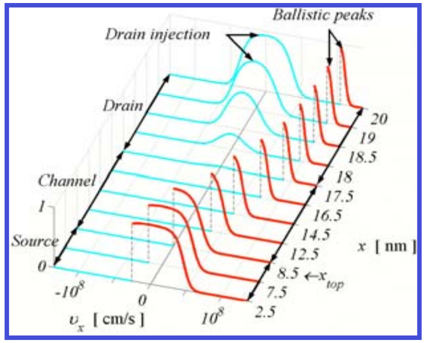
I) Introduction: semiclassical



$$LDOS(x,E) \sim \frac{1}{\sqrt{E - E_C(x)}}$$

I) Introduction: semiclassical ballistic transport





$$n(x_0) = \int \left[LDOS_1(E,x_0)\,f\left(E_{F1}\right) + LDOS_2(E,x_0)\,f\left(E_{F2}\right)\right]dE$$

$$I_D = \frac{2q}{h}\int T(E)\left[f\left(E_{F1}\right) - f\left(E_{F2}\right)\right]dE$$

1) Introduction
2) **Solving the Wave Equation**
3) Computing n(x)
4) Computing I_D
5) Discussion
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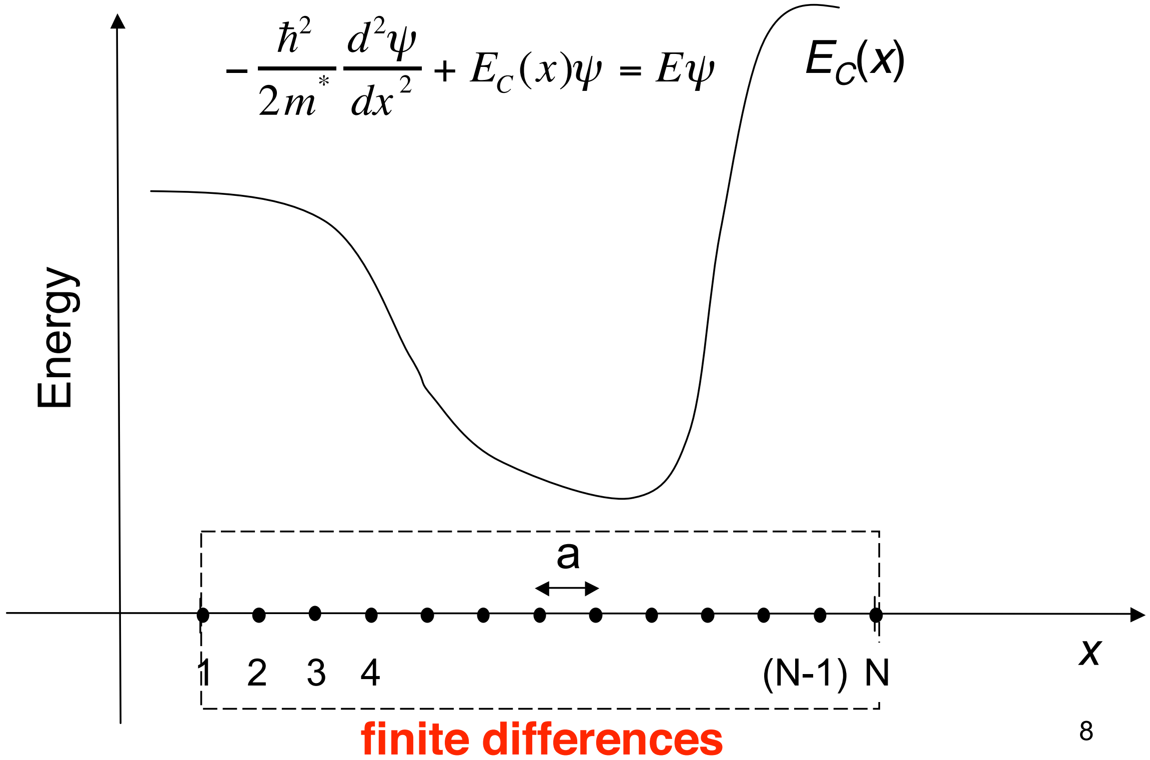
II) Solving the Wave Equation

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$$

$$\begin{cases} -\dfrac{\hbar^2}{2m^*}\dfrac{d^2\psi}{dx^2} + E_C(x)\psi = E\psi \\[2ex] \dfrac{d^2\psi}{dx^2} + k^2\psi = 0 \\[2ex] k \equiv \dfrac{\sqrt{2m^*\left[E - E_C(x)\right]}}{\hbar} \end{cases}$$

II) Solving the Wave Equation: Bound States

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi}{dx^2} + E_C(x)\psi = E\psi$$

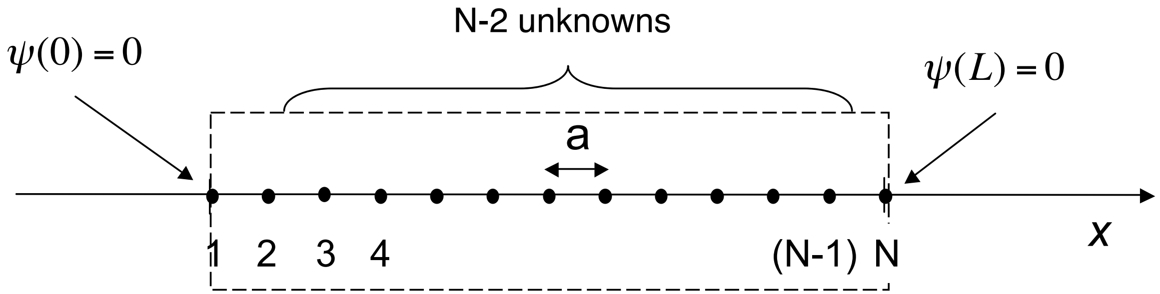


II) Solving the Wave Equation: Discretization

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi}{dx^2} + E_C(x)\psi = E\psi \qquad \left[-t_0\psi_{i-1} + \left(2t_0 + E_{Ci}\right)\psi_i - t_0\psi_{i+1}\right] = E\psi_i$$

i = 2, 3….N-1

$$\left.\frac{d^2\psi}{dx^2}\right|_i = \frac{\psi_{i-1} - 2\psi_i + \psi_{i+1}}{a^2} \qquad t_0 \equiv \frac{\hbar^2}{2m^* a^2}$$

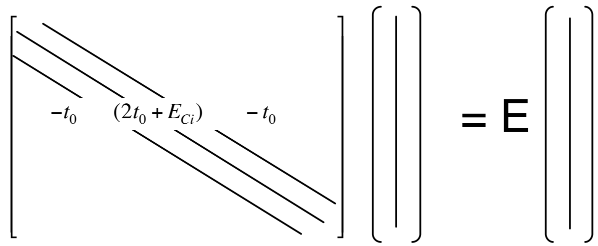


II) Solving the Wave Equation

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

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

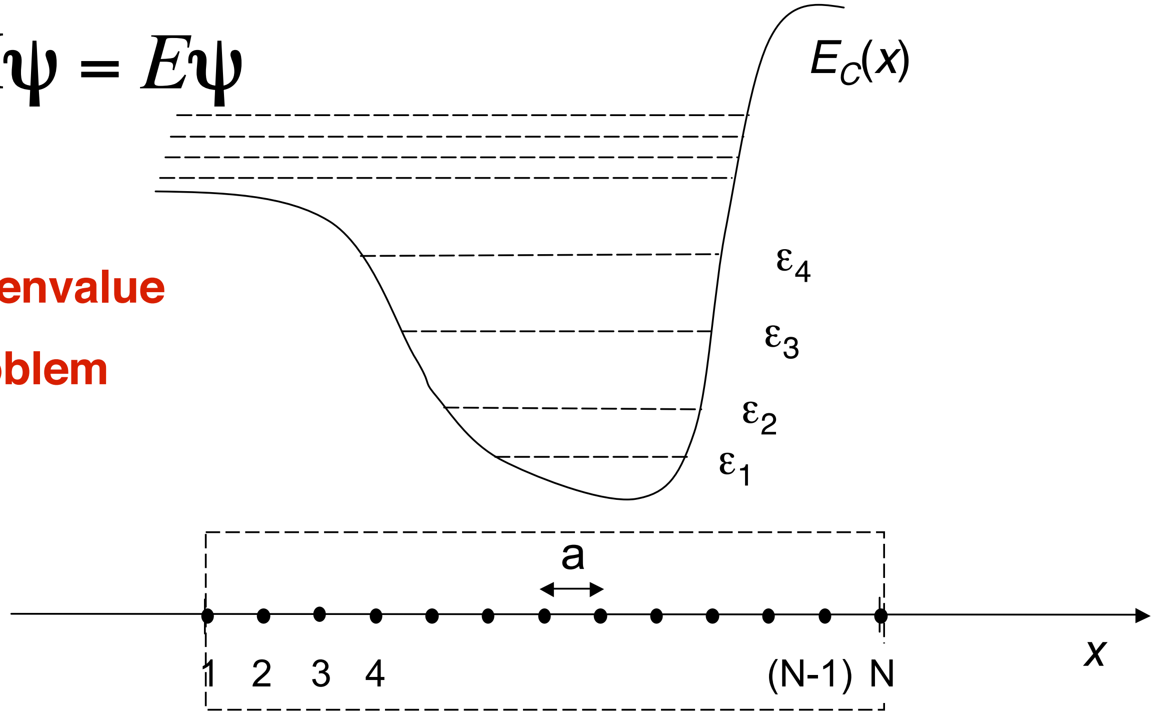
N-2 x N-2 (N-2) x 1



II) Solving the Wave Equation

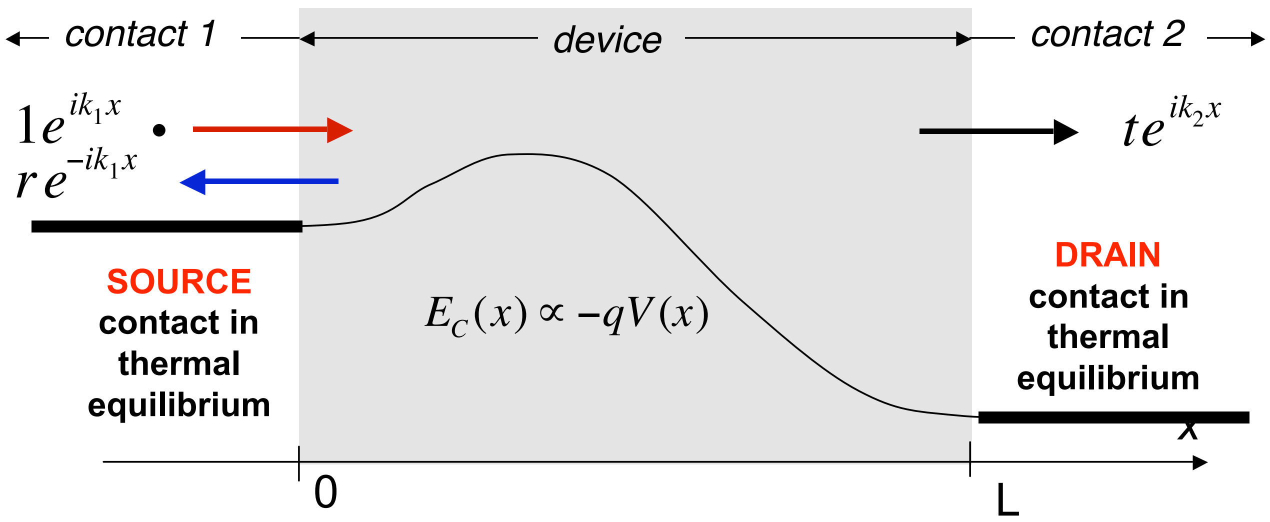
$$\mathbf{H}\psi = E\psi$$

eigenvalue problem



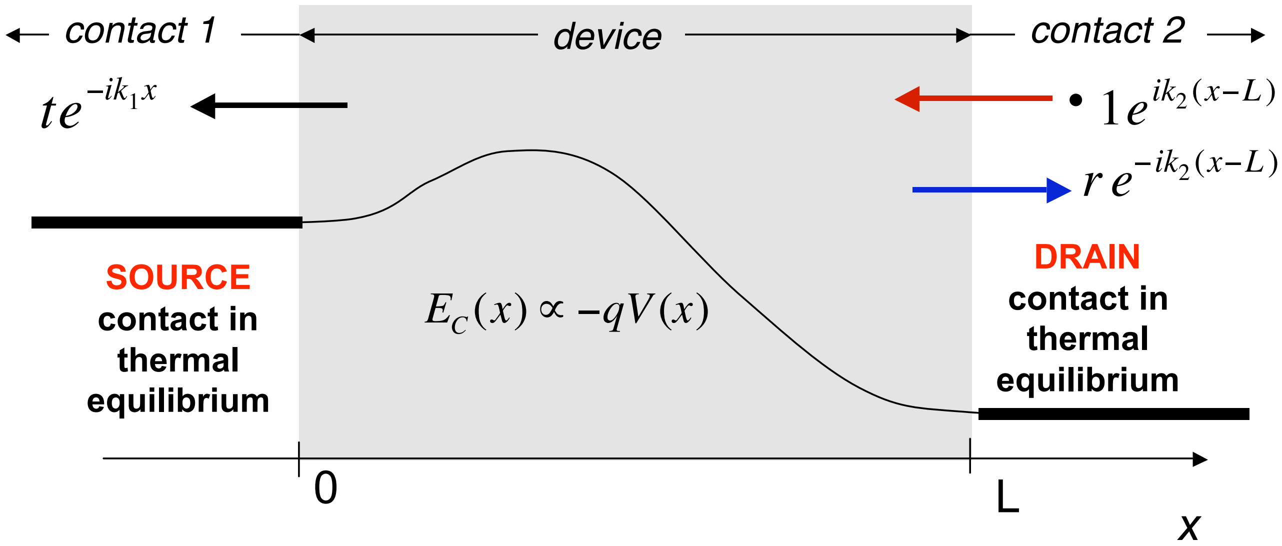
II) Solving the Wave Equation: open systems

source injection: "scattering states"

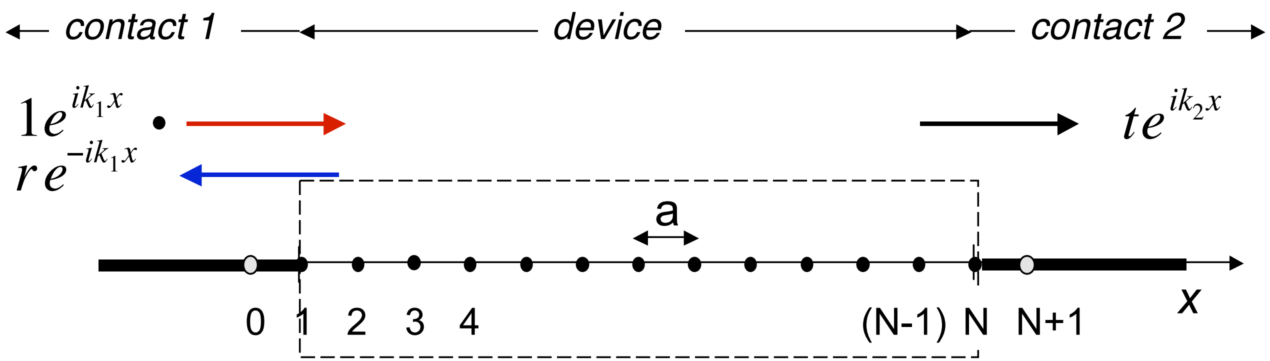


II) Solving the Wave Equation

drain injection: “scattering states”



II) Solving the Wave Equation: A 1D Device



$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi}{dx^2} + E_C(x)\psi = E\psi$$

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

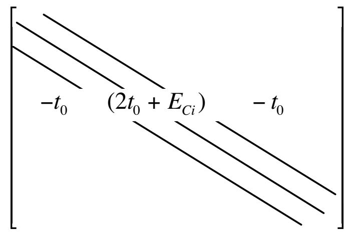
$$\left(E - \hat{H}\right)\psi = 0$$

II) Solving the Wave Equation

$$E\psi_i - \left[-t_0\psi_{i-1} + \left(2t_0 + E_{Ci}\right)\psi_i - t_0\psi_{i+1}\right] = 0 \quad \text{(i = 1, 2…N)}$$

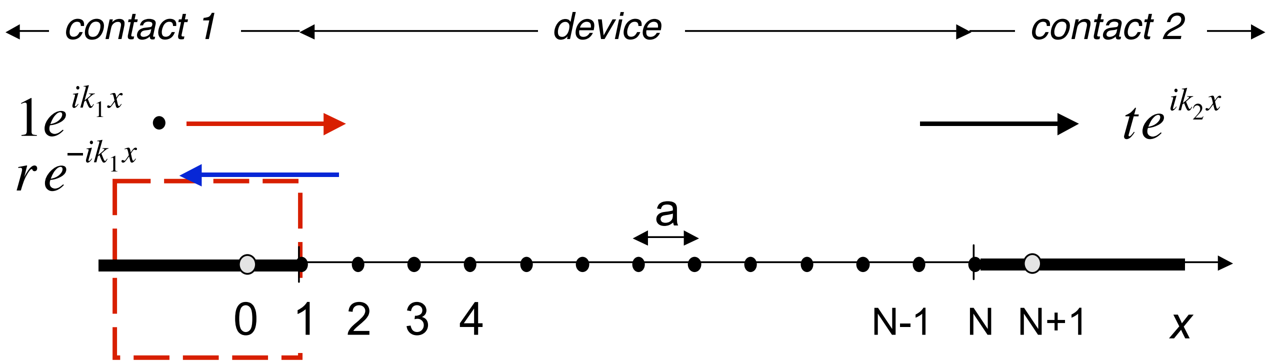
$$\left(E\mathbf{I} - \mathbf{H}\right)\boldsymbol{\psi} = 0$$

N x N   N x 1



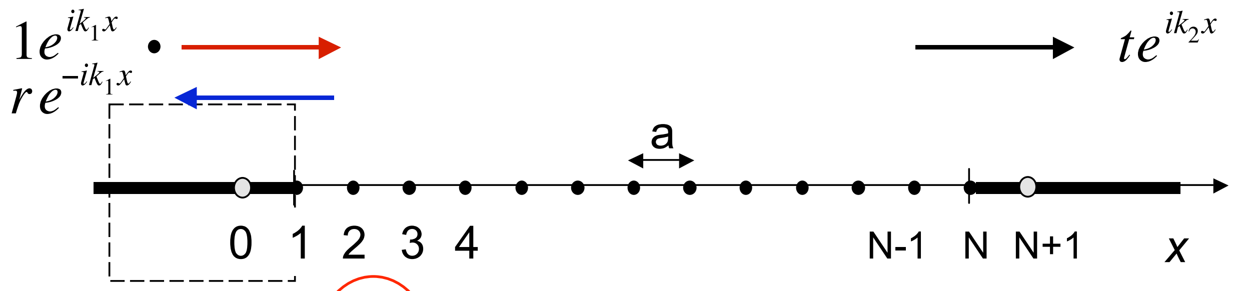
but there is a **problem** at the first node (i = 1) and the last node, (i = N) because they couple to nodes outside the device.

II) Solving the Wave Equation: Open boundary conditions



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

II) Solving the Wave equationn: Treatment of i = 1



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

$$\psi(x) = 1e^{ik_1x} + re^{-ik_1x} \qquad x \le 0$$

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

$$\psi(x=-a) = \psi_0 = e^{-ik_1a} + re^{ik_1a}$$

II) Solving the Wave Equation: Open boundary conditions

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

$$\psi_0 = \psi_1 e^{ik_1 a} - \left(e^{ik_1 a} - e^{-ik_1 a}\right)$$

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

1) add $-t_0 e^{ik_1 a}$ to the diagonal

2) add $t_0\left(e^{ik_1 a} - e^{-ik_1 a}\right)$ to the first column of the RHS

II) Solving the Wave Equation

$$\left[E\mathbf{I} - \mathbf{H} - \sum\nolimits_1 - \sum\nolimits_2\right]\psi = \mathbf{S} = i\gamma$$

$$\begin{bmatrix} \ddots & \ddots & & 0 \\ -t_0 & (2t_0 + E_{C1}) & -t_0 & \\ 0 & \ddots & \ddots & \ddots \end{bmatrix}$$

N x N Hamiltonian

$$\begin{bmatrix} -t_0 e^{ik_1 a} & & \\ & 0 & \\ & & \end{bmatrix} \qquad \begin{bmatrix} & & \\ & 0 & \\ & & -t_0 e^{ik_2 a} \end{bmatrix}$$

N x N lead "self-energies"

$$\begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \\ \psi_N \end{bmatrix}$$

N x 1 wavefunction

$$\begin{bmatrix} -\left[\Sigma_1(1,1) - \Sigma_1^*(1,1)\right] \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

N x 1 "broadening"

II) Solving the wave Equation: The solution

$$\left[E\mathbf{I} - \mathbf{H} - \Sigma_1 - \Sigma_2\right]\psi = \mathbf{S}$$

(not an eigenvalue problem - energy continuous)

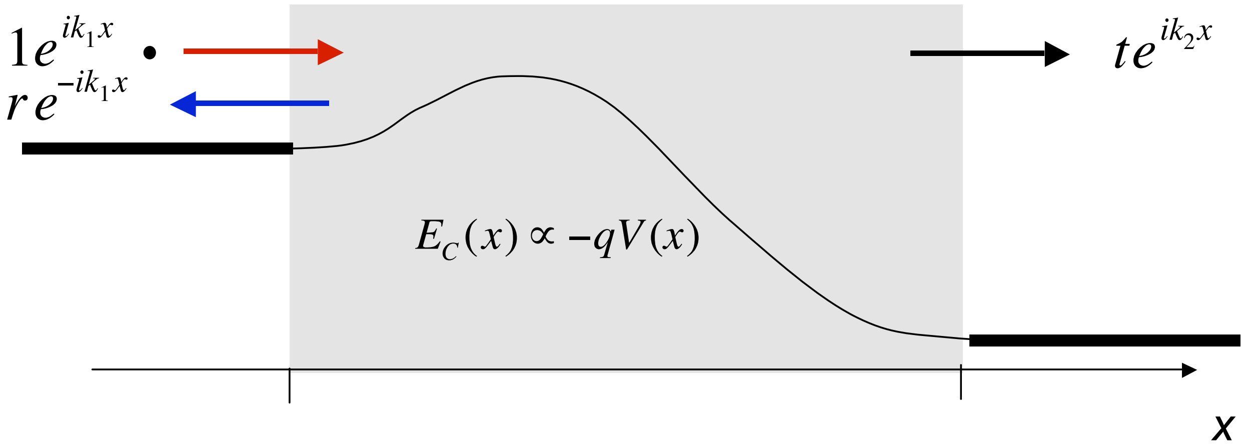
formal solution:

$$\psi = \mathbf{G}^R \mathbf{S}$$

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

(N x N retarded Green's function)

II) Solving the Wave Equation: The self-energies and k



$$\Sigma_1 = \begin{bmatrix} -t_0 e^{ik_1 a} & \\ & 0 \end{bmatrix}$$

$$E - E_{C0} = \hbar^2 k^2 / 2m^*$$

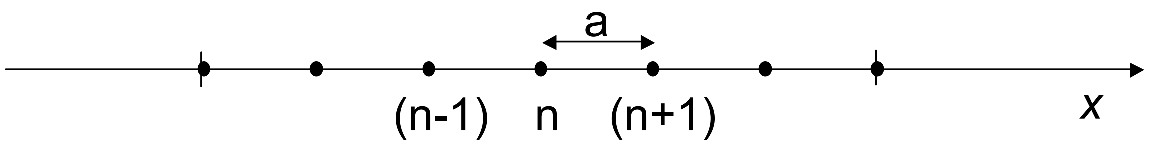
$$k_1 = \sqrt{2m\left(E - E_{C0}\right)} / \hbar$$

$$k_2 = \sqrt{2m\left(E - E_{CL}\right)} / \hbar$$

there is NO E(k) in the device! k refers to the lead

II) Solving the Wave Equation: E_k in the leads

infinite lead



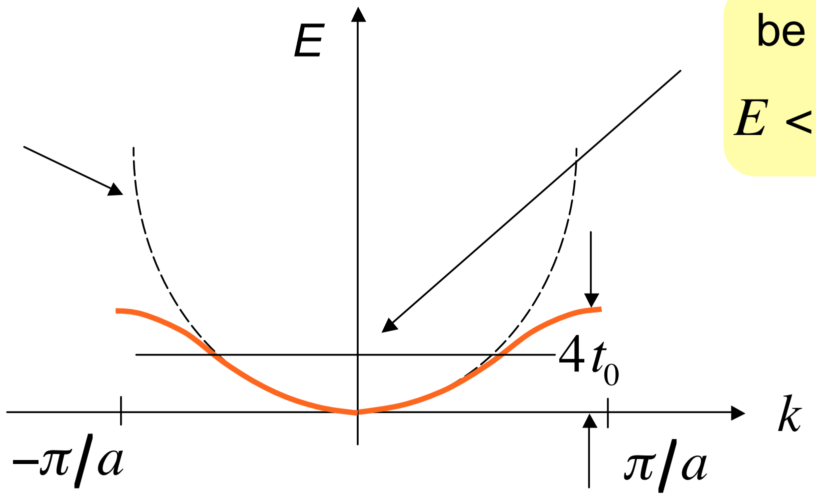
$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi}{dx^2} + E_C\psi = E\psi \quad \Rightarrow \quad -\frac{\hbar^2}{2m^*}\left[\frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{a^2}\right] = \left(E - E_C\right)\psi_n$$

$$\psi_n = e^{ikna} \quad \Rightarrow \quad E_k = E_C + 2t_0\left(1 - \cos ka\right)$$

$$t_0 \equiv \frac{\hbar^2}{2m^* a^2}$$

II) Solving the Wave Equation: E_k in the leads

$$E_k = \frac{\hbar^2 k^2}{2m^*}$$



be sure!

$$E << 4t_0$$

$$E = E_C + 2t_0\left(1 - \cos ka\right)$$

$$t_0 \equiv \frac{\hbar^2}{2m^* a^2}$$

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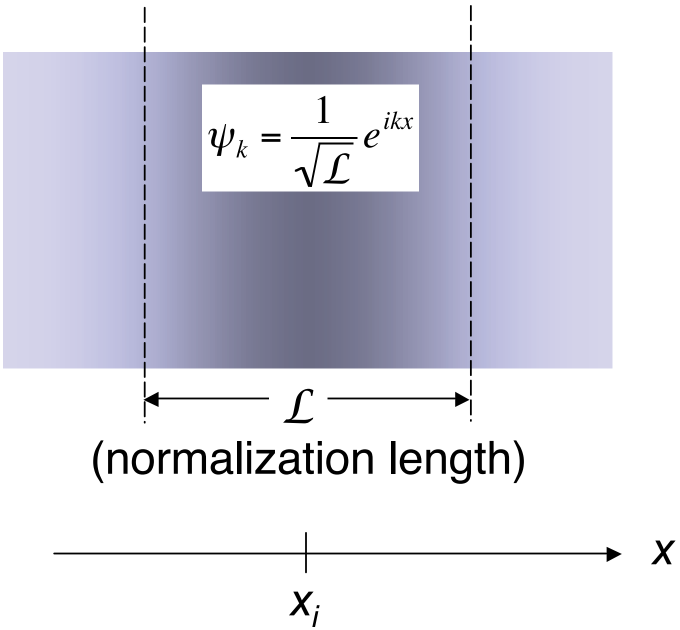
III) Computing n(x): in the bulk

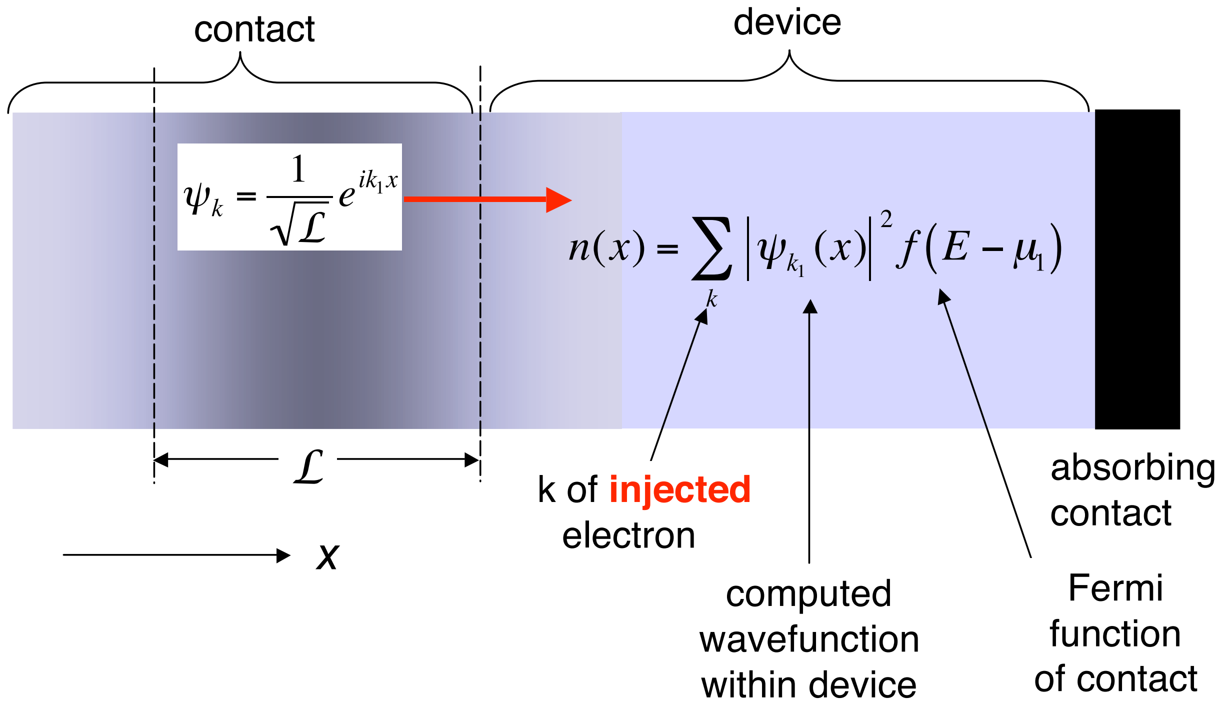


$$n(x_i) = \sum_k \left|\psi_k(x_i)\right|^2 f\left(E-\mu\right)$$

$$n(x_i) = \frac{1}{\mathcal{L}} \sum_k f\left(E-\mu\right)$$

III) Computing n(x)

now attach a device to a bulk contact .....



III) Computing n(x)

sum over the distribution of injected k's from source contact

$$n_1(x_i) = \frac{1}{\mathcal{L}} \sum_{k_1} \left| \psi_{k_1}(x_i) \right|^2 f\left(E - \mu_1\right)$$

normalization length in the **contact**

$$\psi_k = \frac{1}{\sqrt{\mathcal{L}}} e^{ik_1 x}$$

computed assuming unit amplitude injected wave

weight by Fermi function of the source

III) Computing n(x)

$$n_1(x_i) = \frac{1}{\mathcal{L}} \sum_{k_1 > 0} \left|\psi_{k_1}(x_i)\right|^2 f\left(E - \mu_1\right)$$

$$n_1(x_i) = \frac{1}{\mathcal{L}} \frac{\mathcal{L}}{2\pi} \times 2 \int_0^\infty dE \, \frac{dk_1}{dE} \left|\psi_{k_1}(x_i)\right|^2 f\left(E - \mu_1\right)$$

Electron density in the device due to injection from contact 1.

We can write this as:

III) Computing n(x)

$$n_1(x_i) = \underbrace{\int_0^\infty \left[\frac{1}{\pi}\frac{dk_1}{dE}\left|\psi_{k_1}(x_i)\right|^2\right]}_{LDOS_1(x_i, E_k) \equiv 2 \times \frac{A_1(x_i, E_k)}{2\pi}} f_0\left(E - \mu_1\right) dE$$

this is the **portion** of the local density-of-states within the device due to **injection from the source**.

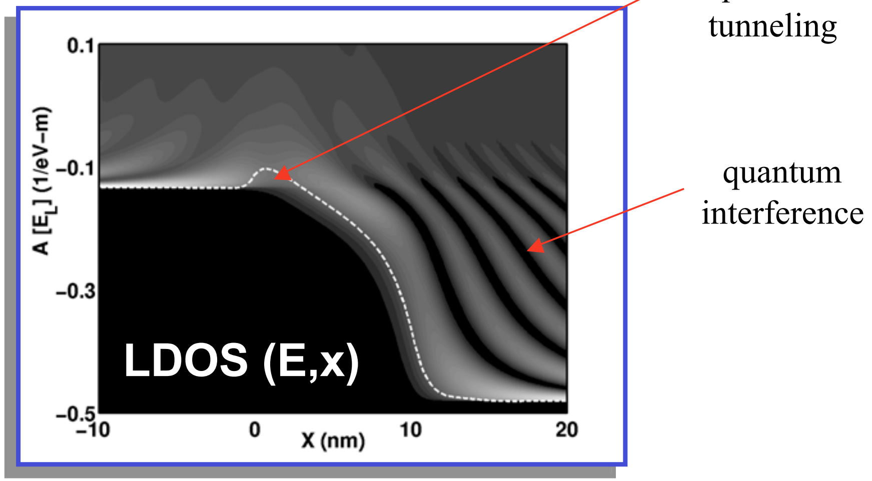
III) Computing n(x)

$$n(x_i) = \int_0^\infty LDOS_1(x_i, E)\, f_0\left(E - \mu_1\right) dE + \int_0^\infty LDOS_2(x_i, E)\, f_0\left(E - \mu_2\right) dE$$

can be computed semi-classically
or
quantum mechanically

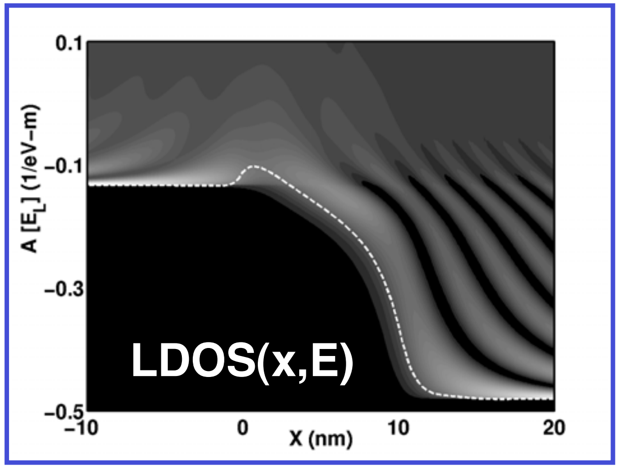
II) Computing n(x): local DOS in a MOSFET

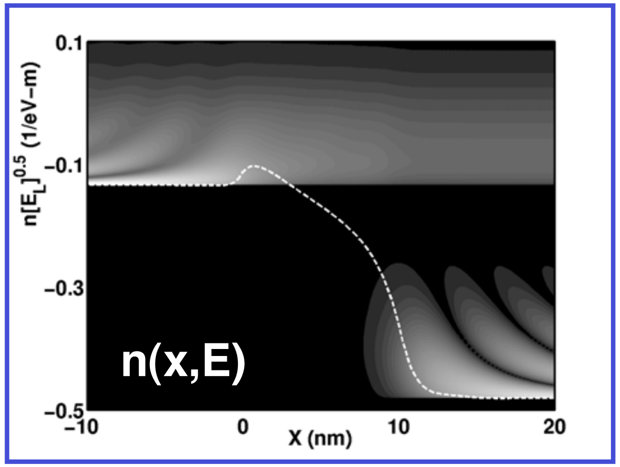
$$LDOS_1(x_i,E) = \left[\frac{1}{\pi}\frac{dk_1}{dE}\left|\psi_{k_1}(x_i)\right|^2\right] \qquad LDOS_2(x_i,E) = \left[\frac{1}{\pi}\frac{dk_2}{dE}\left|\psi_{k_2}(x_i)\right|^2\right]$$



III) Computing n(x)

(on-state, V_{DD} = 0.4 V)



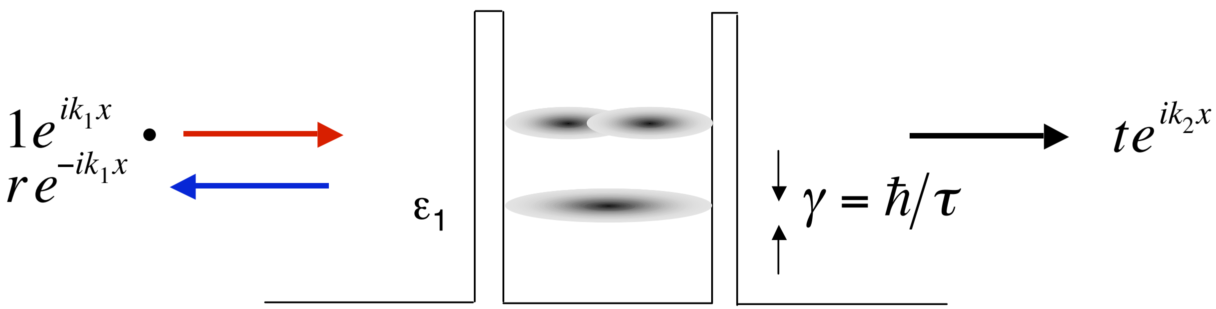


$$LDOS(x,E) = LDOS_1(x,E) + LDOS_1(x,E)$$

$$n_1(x,E) = f_1(E)LDOS_1(x,E)$$

$$n_2(x,E) = f_2(E)LDOS_2(x,E)$$

III) Computing n(x): bound states again



"broadening"

1) Introduction
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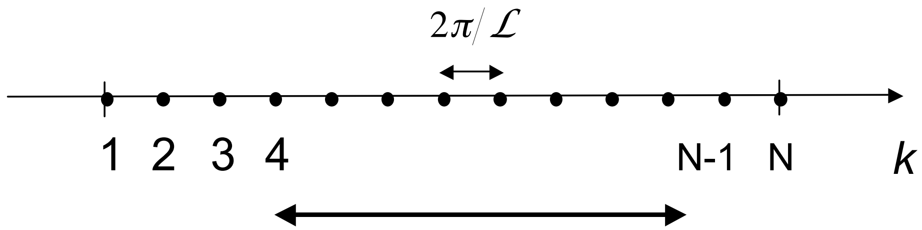
IV) Computing I_D

let's derive the current expression beginning with:

$$I_{1-2} = \frac{q}{\mathcal{L}} \sum_{k>0} T_{1-2}(E)\, \upsilon_k\, f(E-\mu_1)$$



$$\frac{dk}{(2\pi/\mathcal{L})} \times 2$$

states in *dk*

IV) Computing I_D

$$I_{1-2} = \frac{q}{\mathcal{L}} \sum_{k>0} T_{1-2}(E)\upsilon_k\, f(E-\mu_1)$$

$$\sum_{k>0} \bullet \quad \Rightarrow \quad \left(\frac{\mathcal{L}}{\pi}\right)\int_{k>0} \bullet\, dk$$

$$\Rightarrow \quad I_{1-2} = \frac{q}{\pi}\int T_{1-2}(E)\upsilon_k f(E-\mu_1)dk$$

IV) Computing I_D

$$I_{1-2} = \frac{q}{\pi} \int_{k>0} T_{1-2}(E)\,\upsilon_k\, f\left(E-\mu_1\right)dk$$

$$= \frac{q}{\pi} \int_{k>0} T_{1-2}(E)\frac{dE}{d(\hbar k)}\, f\left(E-\mu_1\right)dk$$

$$I_{1-2} = \frac{2q}{h} \int_{0} T_{1-2}(E)\, f\left(E-\mu_1\right)dE$$

IV) Computing I_D

$$I_D = I_{1-2} - I_{2-1}$$

$$\left.\begin{aligned} I_{1-2} &= \frac{2q}{h}\int_0 T_{1-2}(E)\, f(E-\mu_1)\, dE \\ I_{2-1} &= \frac{2q}{h}\int_0 T_{2-1}(E)\, f(E-\mu_2)\, dE \end{aligned}\right\}$$

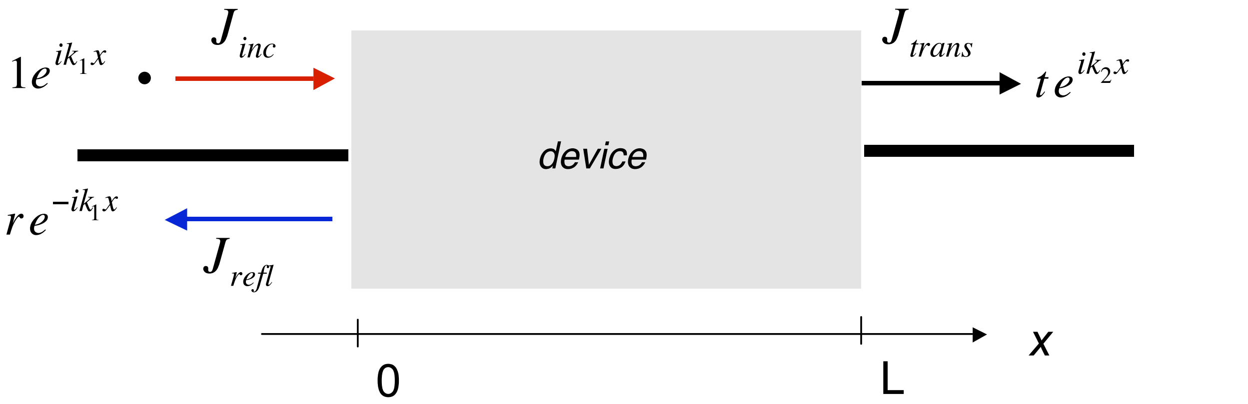
can show:

$$T_{1-2}(E) = T_{2-1}(E)$$

(ballistic)

$$I_D = \frac{2q}{h}\int_0 T(E)\left[f(E-\mu_1) - f(E-\mu_2)\right] dE$$

IV) Computing I_D: Finding $T_{1\text{-}2}(E)$

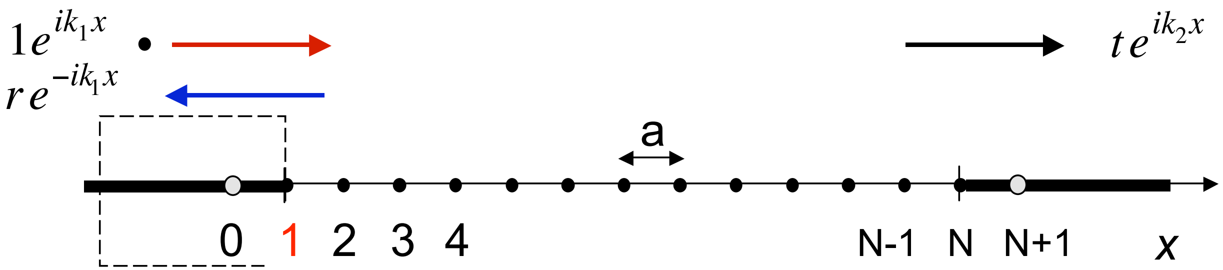


$$J_{trans} = J_{inc} - J_{refl}$$

$$J_{inc} = \frac{\hbar k_1}{m^*} \qquad J_{refl} = \frac{\hbar k_1}{m^*}|r|^2$$

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

IV) Computing I_D: Finding $T_{1\text{-}2}(E)$



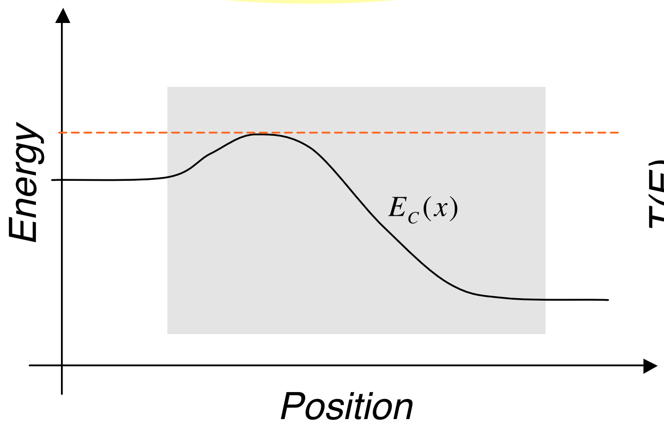
$$\psi(x) = 1e^{ik_1x} + re^{-ik_1x} \qquad x \le 0$$

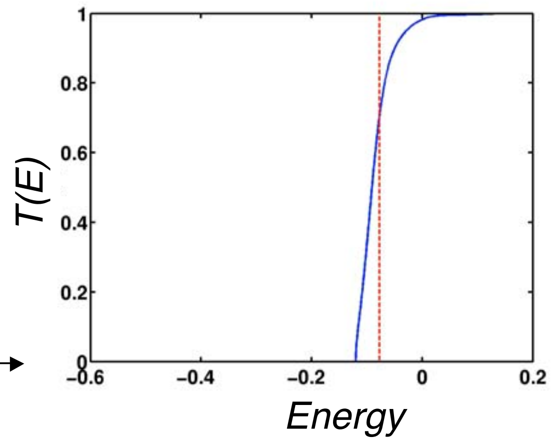
$$\psi(x=0) = 1 + r = \psi_1$$

$$T_{1-2}(E) = 1 - \left|\psi_1 - 1\right|^2$$

IV) Computing I_D: $T_{1\text{-}2}(E)$ for a MOSFET

$$T_{1-2}(E) = 1 - \left|\psi_1 - 1\right|^2$$





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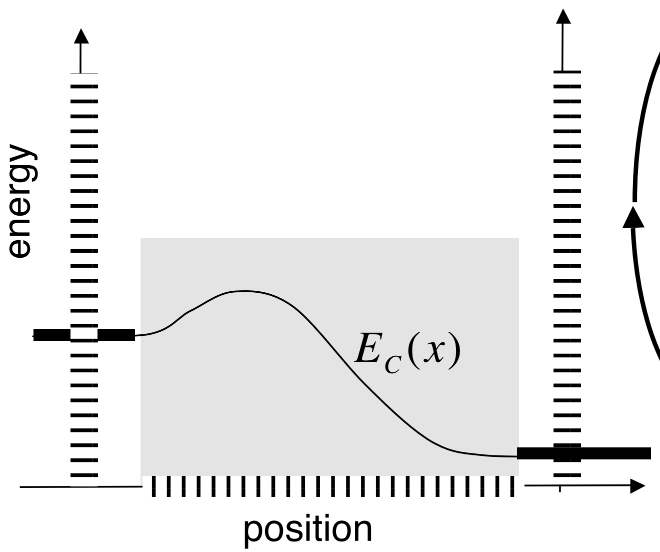
V) Discussion: The wavefunction approach



1) Guess $E_C(x)$
2) For each energy:

$$\left[E\mathbf{I}-\mathbf{H}-\Sigma_1-\Sigma_2\right]\psi=\mathbf{S}$$

3) Determine $n(x)$:

$$n(x_i)=n_1(x_i)+n_2(x_i)$$

4) solve Poisson for $E_C(x)$
5) go to 1

6) Determine I_D

$$I_D=I_{1-2}-I_{2-1}$$

V) Discussion: Key Results

$$\left[E\mathbf{I}-\mathbf{H}-\Sigma_1-\Sigma_2\right]_{\mathrm{NxN}}\psi_{\mathrm{Nx1}}=i\gamma_{\mathrm{Nx1}}$$

$$n_1(x_i)=\int_0^{E_{Top}}2\times\frac{A_1(E_k,x_i)}{2\pi}f\left(E_F-E_k\right)dE_k$$

$$\frac{A_1(x_i,E)}{2\pi}=\left(\frac{1}{2\pi}\frac{dk}{dE}\left|\psi_k(x_i)\right|^2\right)$$

$$I^{1-2}=\frac{2q}{h}\int_0^{E_{Top}}T(E)f\left(E_k\right)dE_k$$

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

$$\boldsymbol{\psi}_{\mathbf{Nx1}}=i\,\mathbf{G}_{\mathrm{NxN}}\gamma_{\mathrm{Nx1}}$$

$$\mathbf{G}_{\mathrm{NxN}}=\left[E\mathbf{I}-\mathbf{H}-\Sigma_1-\Sigma_2\right]_{\mathrm{NxN}}^{-1}$$

Can we do everything with the Green's function?

V) Discussion: density matrix

We need $\psi^* \psi$ at each node. $\boldsymbol{\psi\psi}^H = \left(\mathbf{G}\boldsymbol{\gamma}_1\right)\left(\boldsymbol{\gamma}_1^{\mathbf{H}}\mathbf{G}^{\mathbf{H}}\right)$

We have:

$$\boldsymbol{\psi} = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \\ \\ \\ \psi_N \end{bmatrix} \qquad \begin{pmatrix} \psi_1^*\psi_1 & \psi_1^*\psi_2 & \psi_1^*\psi_3 & \cdots & \\ \psi_2^*\psi_1 & \psi_2^*\psi_2 & & & \\ \psi_3^*\psi_1 & & \psi_3^*\psi_3 & & \\ \vdots & & & \ddots & \\ & & & & \psi_N^*\psi_N \end{pmatrix}$$

V) Discussion: density matrix

(N x 1) $$n_1(x_i) = \int_0^{E_{Top}} \frac{1}{\pi}\frac{dk}{dE_k}\left|\psi_k(x_i)\right|^2 f\left(E_k\right)dE$$

(N x N) $$\rho_1 = \int_0^{E_{Top}} \frac{1}{\pi}\frac{dk}{dE_k}\left\{\mathbf{G}\gamma_1\gamma_1^{\mathbf{H}}\mathbf{G}^{\mathbf{H}}\right\}f\left(E\right)dE$$

$$\gamma_1 = \begin{bmatrix} i\left[\Sigma_1(1,1) - \Sigma_1^*(1,1)\right] \\ \vdots \\ \\ 0 \end{bmatrix} = \begin{bmatrix} 2t_0 \sin ka \\ \vdots \\ \\ 0 \end{bmatrix}$$

$$\gamma_1\gamma_1^H = \begin{bmatrix} 4t_0^2 \sin^2 ka & \cdots & 0 \\ \vdots & \ddots & \\ \\ 0 & & 0 \end{bmatrix}$$

V) Discussion: density matrix

$$\rho_1 = \int_0^{E_{Top}} \frac{1}{\pi}\frac{dk}{dE_k}\left\{\mathbf{G}\gamma_1\gamma_1^{\mathbf{H}}\mathbf{G}^{\mathbf{H}}\right\} f(E)\,dE$$

$$E(k) = 2t_0(1-\cos ka)$$

$$\frac{dk}{dE} = \frac{1}{2at_0\sin ka}$$

$$\gamma_1\gamma_1^H = \begin{bmatrix} 4t_0^2\sin^2 ka & \cdots & 0 \\ \vdots & \ddots & \\ 0 & & 0 \end{bmatrix}$$

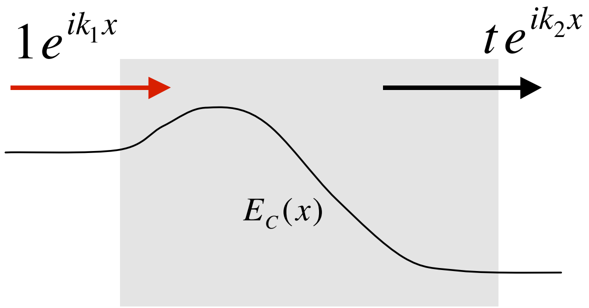
V) Discussion: spectral function

$$\frac{a}{\pi}\frac{dk}{dE}\gamma\gamma^{\mathrm{H}} \equiv \mathbf{\Gamma}_1 = \begin{bmatrix} 2t_0 \sin ka & \cdots & 0 \\ \vdots & \ddots & \\ & & \\ 0 & & 0 \end{bmatrix} = i\left(\mathbf{\Sigma}_1 - \mathbf{\Sigma}_1^{H}\right)$$

$$\boldsymbol{\rho}_1 \Big|_{\mathrm{NxN}} = \int 2 \times \frac{\mathbf{A_1}\big|_{\mathrm{NxN}}}{2\pi} f\left(E_F - E\right) dE$$

$$\mathbf{A_1} = \mathbf{G}\mathbf{\Gamma}_1\mathbf{G}^{\mathbf{H}}$$

V) Discussion: transmission



$$J_{inc} = 1\upsilon_1$$

$$J_{trans} = |t|^2 \upsilon_N$$

$$T = |t|^2 \left(\frac{\upsilon_N}{\upsilon_1}\right)$$

$$\upsilon_1 = \frac{2at_0}{\hbar}\sin k_0 a = \left(\frac{a}{\hbar}\right)\Gamma_1(1,1) \qquad |t|^2 = |\psi_N|^2$$

$$\upsilon_N = \frac{2at_0}{\hbar}\sin k_N a = \left(\frac{a}{\hbar}\right)\Gamma_2(N,N) \qquad \psi_N = G(N,1)\Gamma_1(1,1)$$

V) Discussion: transmission

$$T(E) = |t|^2 \frac{\upsilon_N}{\upsilon_1} = |\psi_N|^2 \frac{\Gamma_2(N,N)}{\Gamma_1(1,1)} = \left|G(N,1)\right)\Gamma_1(1,1)\Big|^2 \frac{\Gamma_2(N,N)}{\Gamma_1(1,1)}$$

$$T(E) = G(N,1)\Gamma_1^*(1,1)G^H(N,1)\Gamma_2(N,N)$$

more generally, for transmission from contact 1 to 2:

$$T(E) = \text{trace}\left[\Gamma_1 \mathbf{G}\,\Gamma_2 \mathbf{G}^{\mathrm{H}}\right]$$

V) Discussion: key results in NEGF form

$$\mathbf{G} = \left[E\mathbf{I} - \mathbf{H} - \Sigma_1 - \Sigma_2\right]^{-1}$$

$$\boldsymbol{\rho}_1 = \int 2 \times \frac{dE}{2\pi} \mathbf{A}_1(E) f\left(E_F - E\right)$$

$$\mathbf{A}_1(E) = \mathbf{G}\boldsymbol{\Gamma}_1\mathbf{G}^H$$

$$I^{1-2} = \frac{2q}{h}\int T^{1-2}(E) f\left(E_F - E_k\right) dE$$

$$T^{1-2}(E) = \mathrm{trace}\left[\boldsymbol{\Gamma}_1\mathbf{G}\boldsymbol{\Gamma}_2\mathbf{G}^{\mathrm{H}}\right]$$

$$\boldsymbol{\Sigma}_1 = \begin{bmatrix} -t_0 e^{ik_1 a} & 0 & \ldots \\ 0 & 0 & \ldots \\ \ldots & \ldots & \ldots \end{bmatrix}$$

$$\boldsymbol{\Sigma}_2 = \begin{bmatrix} \ldots & \ldots & \ldots \\ \ldots & 0 & 0 \\ \ldots & 0 & -t_0 e^{ik_N a} \end{bmatrix}$$

$$\boldsymbol{\Gamma}_1 = \boldsymbol{\Sigma}_1 - \boldsymbol{\Sigma}_1^H$$

$$\boldsymbol{\Gamma}_2 = \boldsymbol{\Sigma}_2 - \boldsymbol{\Sigma}_2^H$$

V) Discussion: What else?

1) scattering
2) two and three dimensions
3) atomistic basis
4) boundary conditions
5) many body effects
6) …

1) Introduction
2) Solving the Wave Equation
3) Computing n(x)
4) Computing I_D
5) Discussion
6) **Summary**

1) The NEGF provides a convenient formalism for solving the Schrödinger equation with open boundary conditions.
2) NEGF also provides a rigorous basis for going beyond the single electron Schrödinger equation.
3) NEGF is rapidly becoming an essential tool for device engineers.
4) For more information, see

www.nanohub.org