A Top-Down Introduction to the NEGF Approach

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1) Introduction
2) Solving the Wave Equation
3) Computing n(x)
4) Computing I_D
5) NEGF Formulation
6) Scattering
7) Summary

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I) Introduction: device simulation

(1) "Poisson" Equation

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

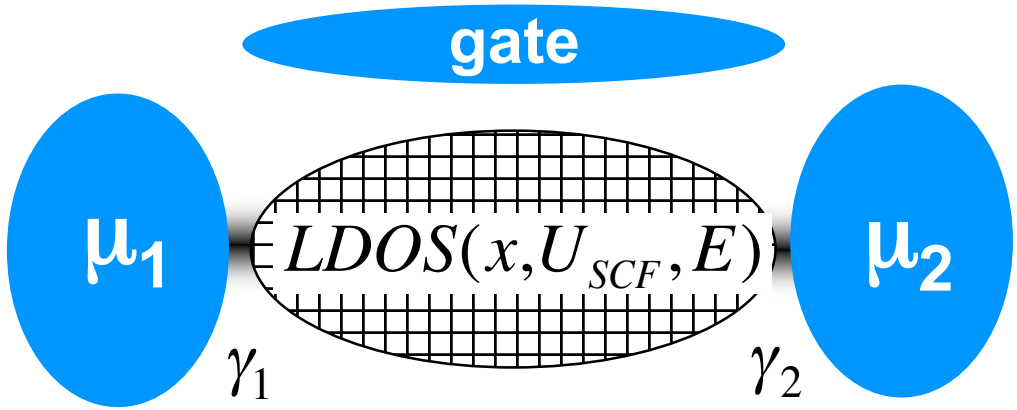
(2) Transport Equation

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

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

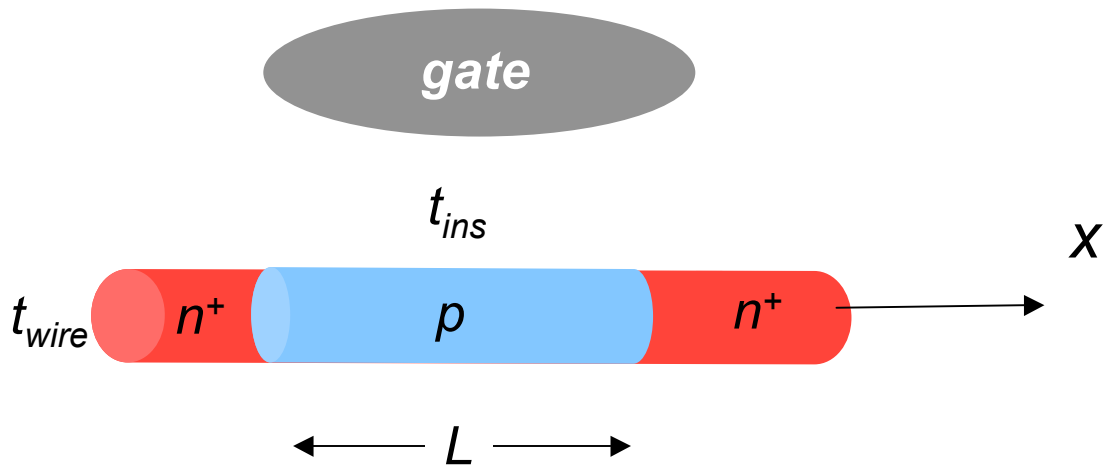
I) Introduction: device simulation

(1) Compute U_{SCF}



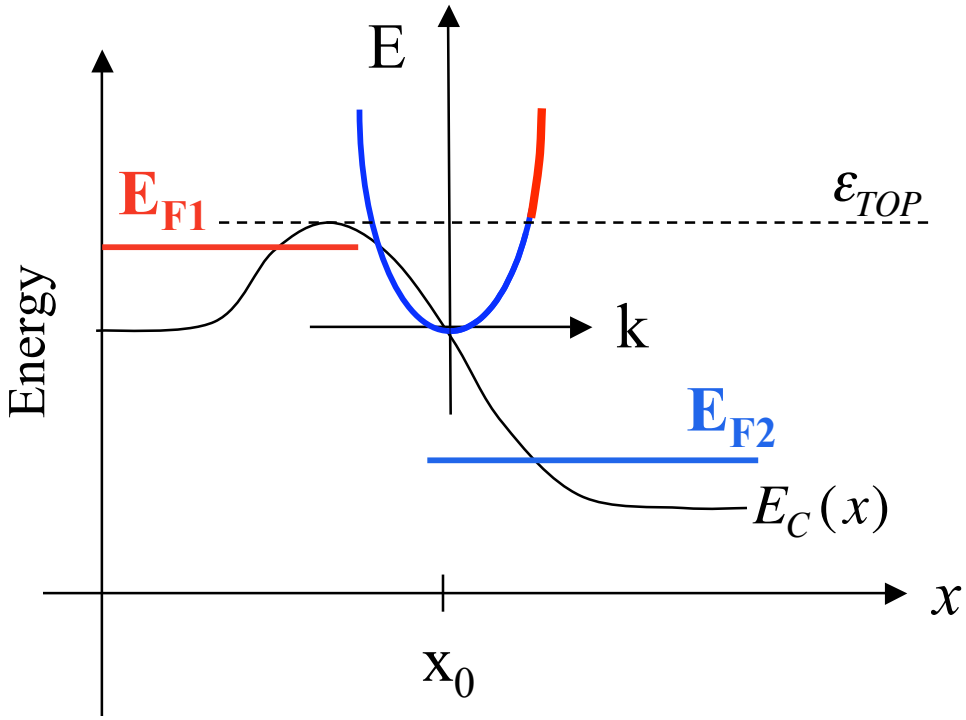
(2) Compute / fill LDOS

(1) 3D electrostatics



(2) 1D transport

I) Introduction: semiclassical approach



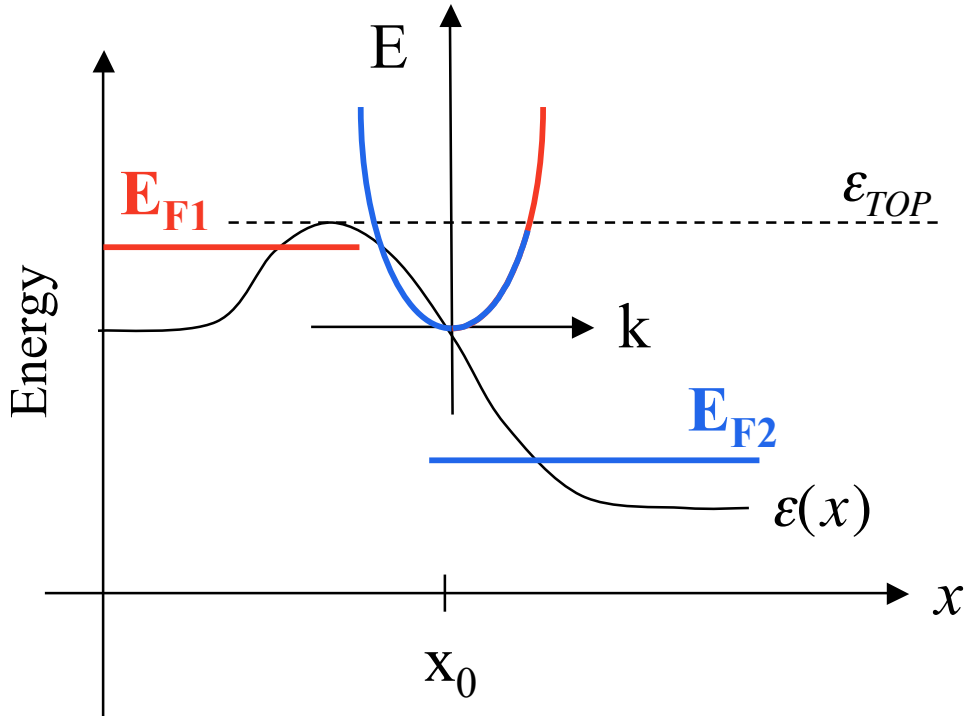
bulk:

$$D(E) \sim \frac{1}{\sqrt{E - E_C}}$$

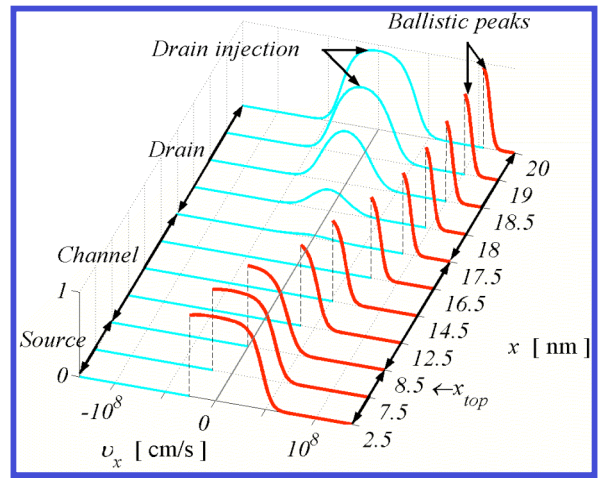
device:

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

I) Introduction: semiclassical ballistic transport



$V_{GS}=V_{DS} = 0.6$



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

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

1) Introduction
2) **Solving the Wave Equation**
3) Computing n(x)
4) Computing I_D
5) NEGF Formulation
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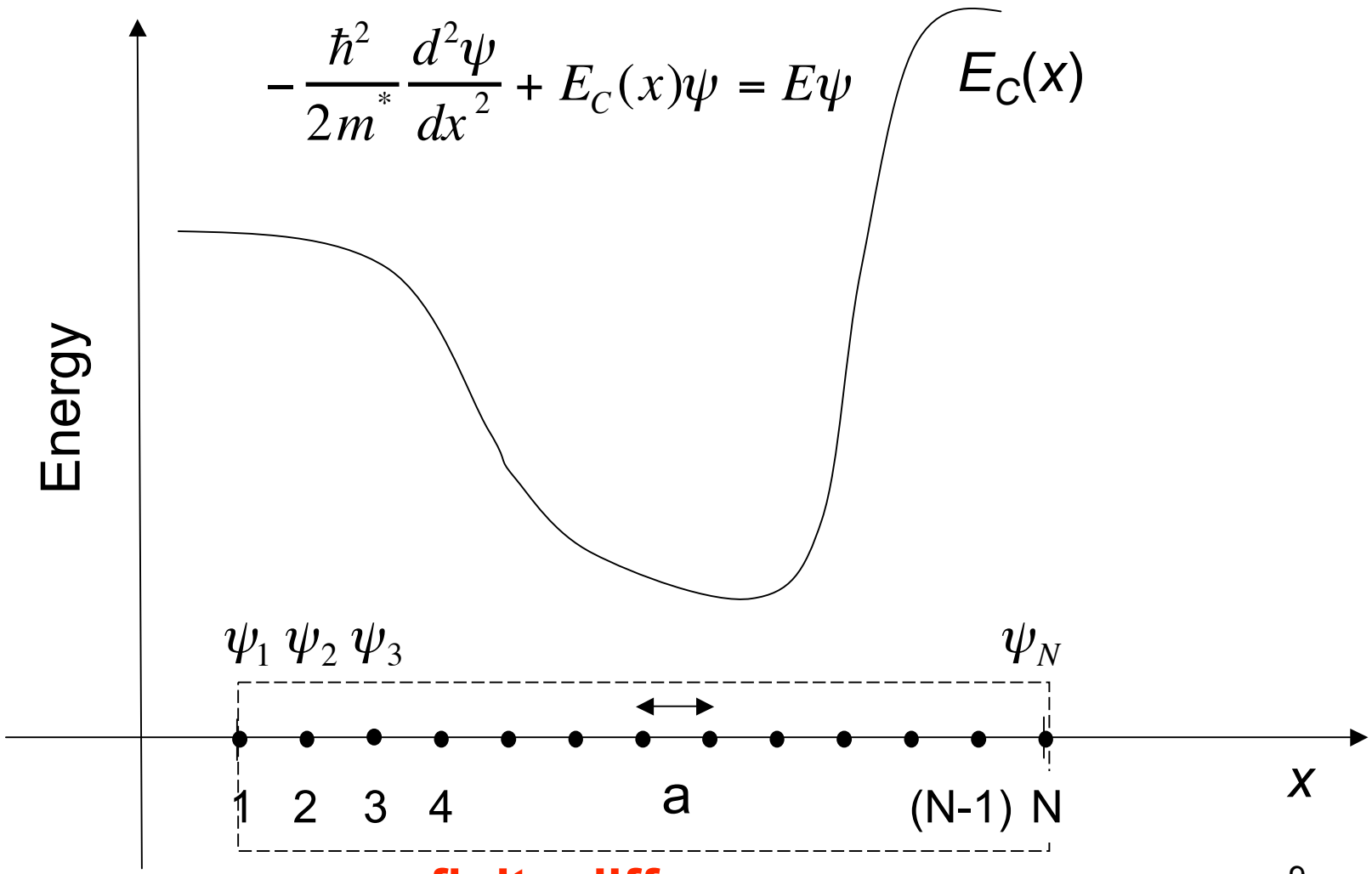
II) Solving the Wave Equation: steady-state

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

II) Solving the Wave Equation: Bound States

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



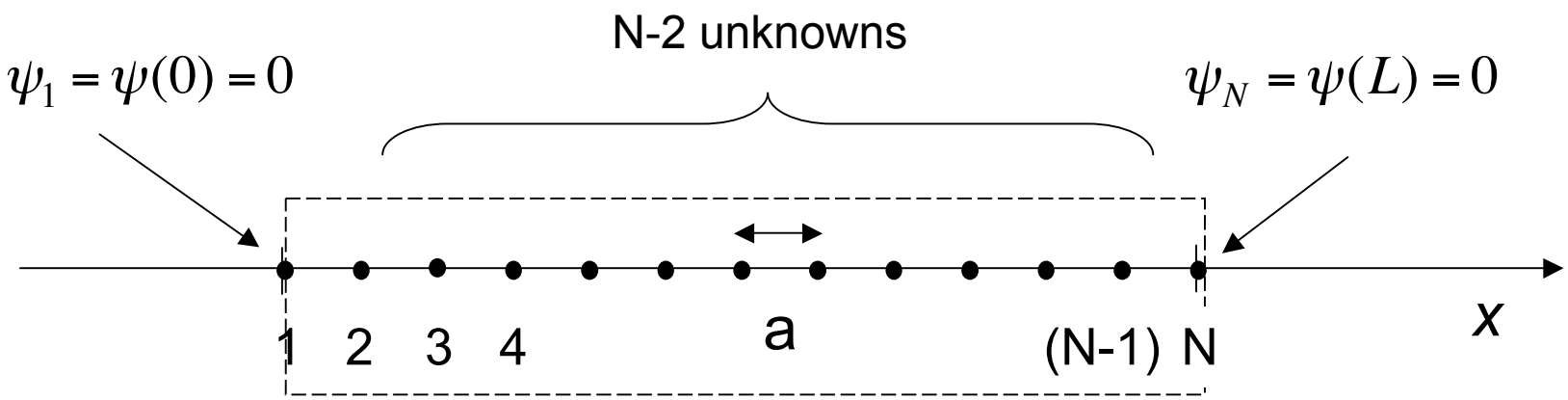
finite differences

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

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

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

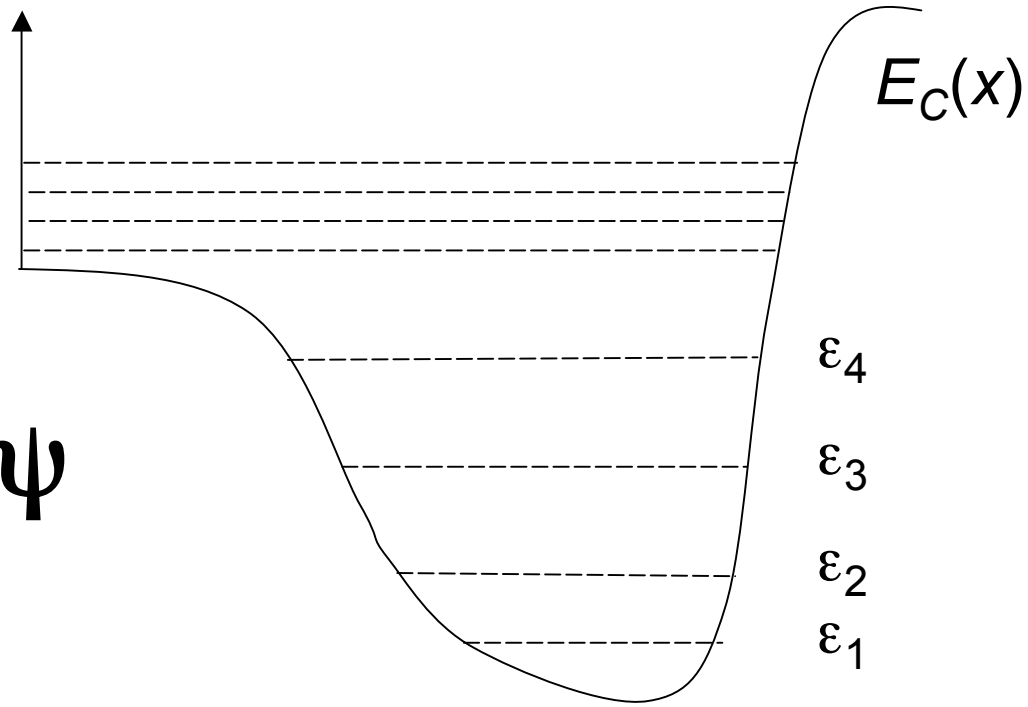
$$\begin{bmatrix} \ddots & \ddots & \ddots & & \\ -t_0 & (2t_0 + E_{Ci}) & -t_0 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots \end{bmatrix} \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_{N-1} \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_{N-1} \end{pmatrix}$$

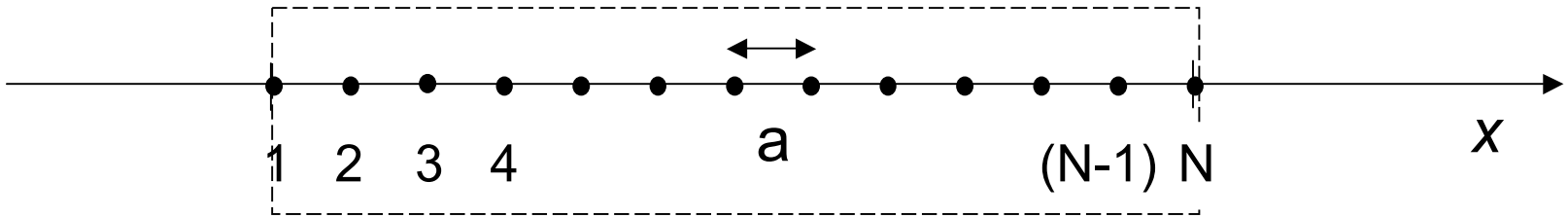
N-2 x N-2 (N-2) x 1 (N-2) x 1

II) Solving the Wave Equation

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

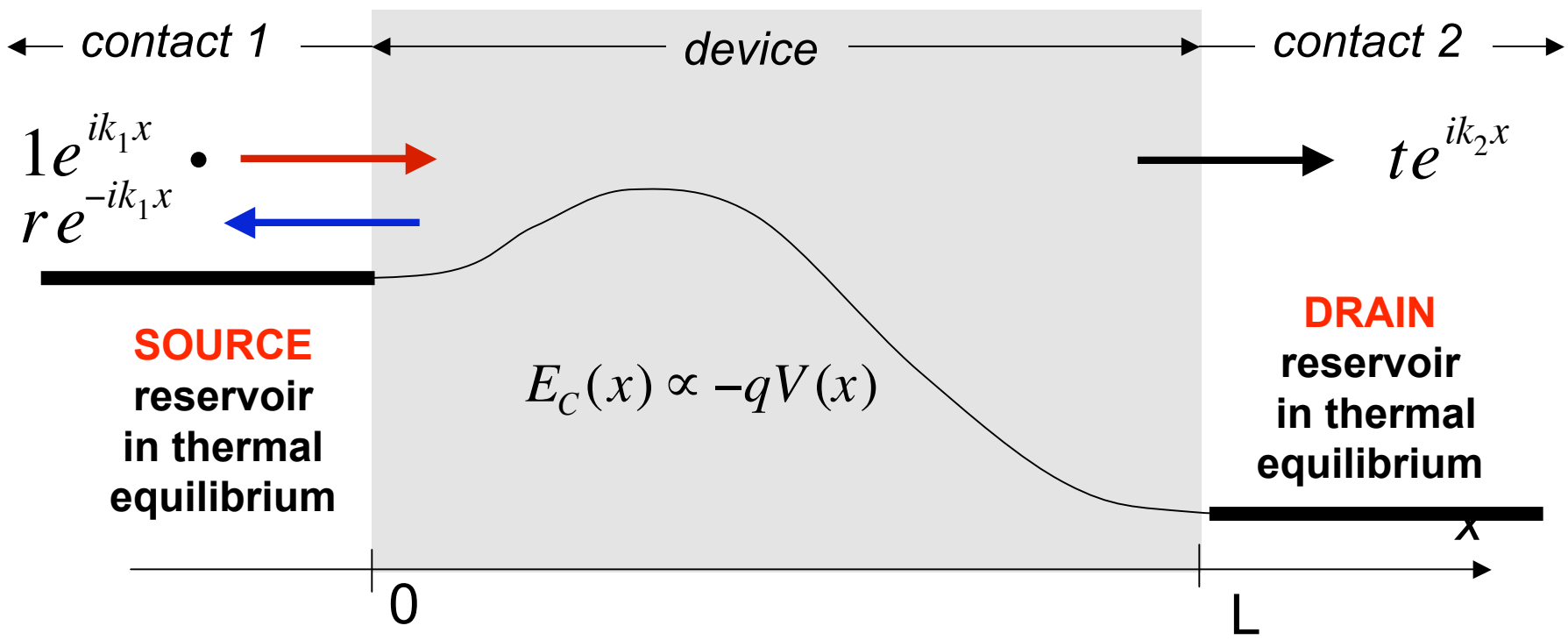
eigenvalue problem





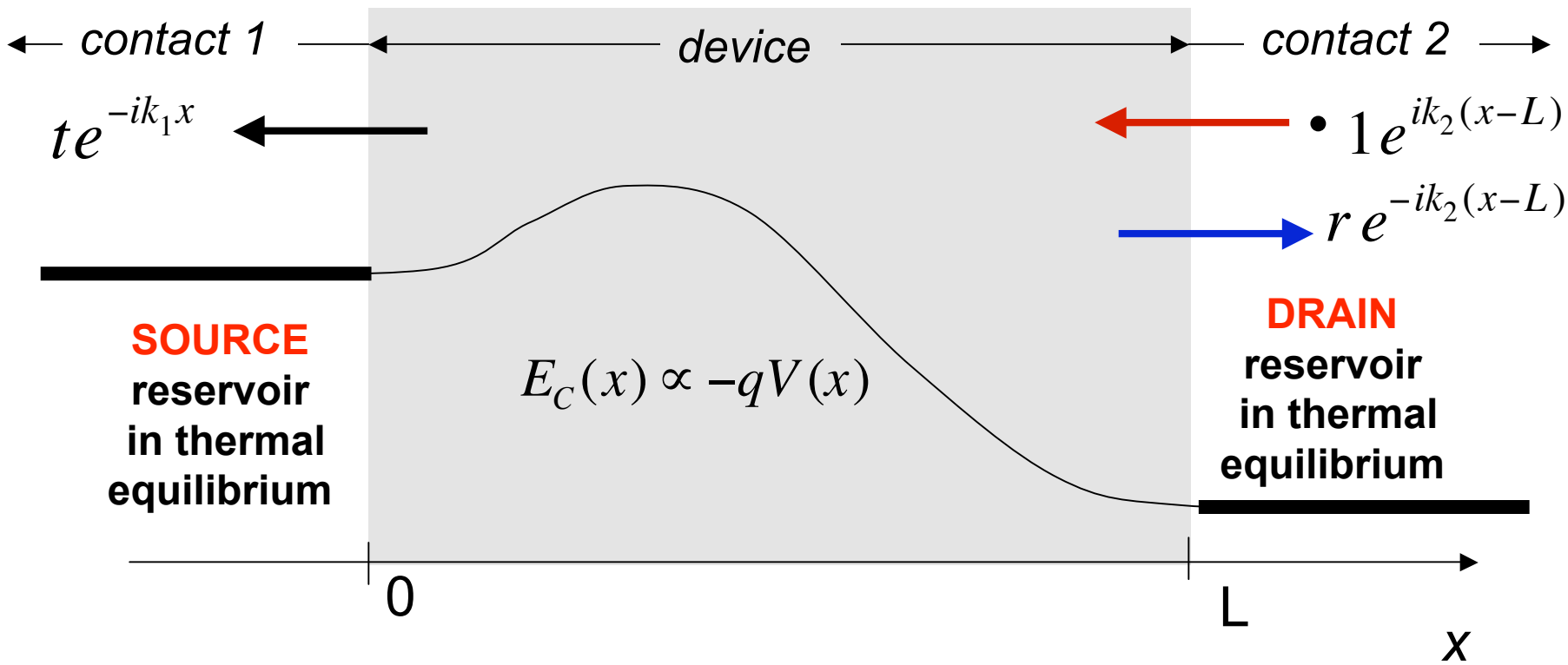
II) Solving the Wave Equation: open systems

source injection: "scattering states"

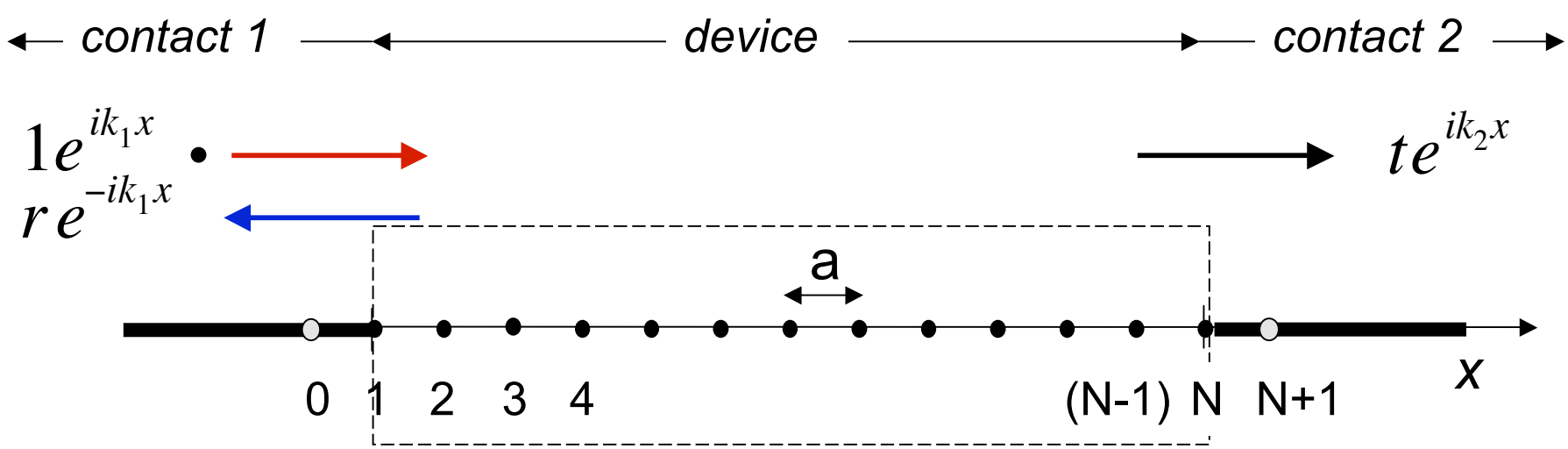


II) Solving the Wave Equation

drain injection: "scattering states"



II) Solving the Wave Equation: A 1D Device



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

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

II) Solving the Wave Equation

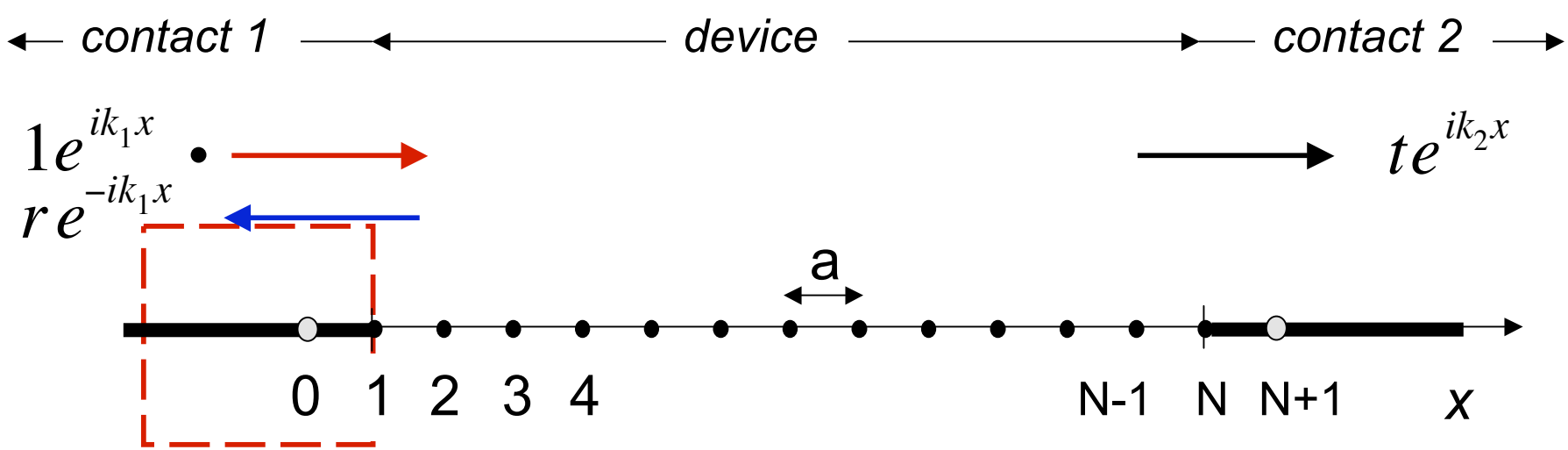
$$E\psi_i - \left[-t_0\psi_{i-1} + \left(2t_0 + E_{Ci}\right)\psi_i - t_0\psi_{i+1}\right] = 0 \quad \text{(i = 1, 2…N)}$$

$$\left(E\mathbf{I} - \mathbf{H}\right)\boldsymbol{\psi} = 0 \qquad \mathbf{H} = \begin{bmatrix} \ddots & \ddots & \ddots & & \\ -t_0 & (2t_0 + E_{Ci}) & -t_0 & & \\ & \ddots & \ddots & \ddots & \\ & & & & \end{bmatrix}$$

N x N N x 1

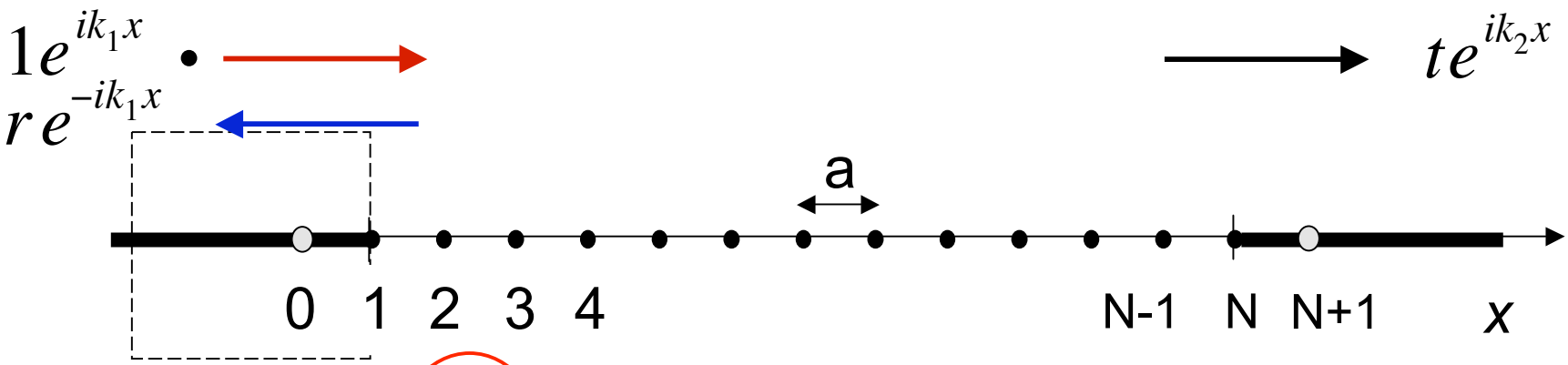
but there is a **problem** at the first node (i = 1) and the last node, (i = N) because they couple to nodes outside the device.

II) Solving the Wave Equation: Open boundary conditions



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

II) Solving the Wave equation: 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

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

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

N x N Hamiltonian

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

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

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)

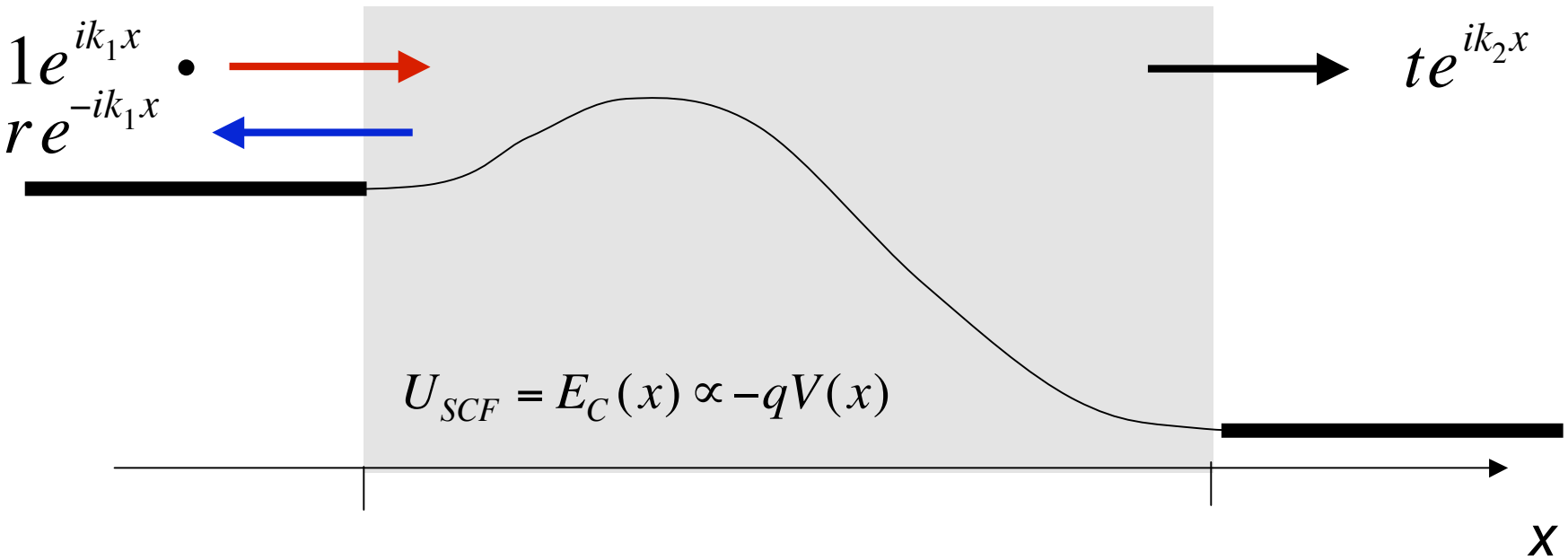
formal solution:

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

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

(N x N retarded Green's function)

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



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

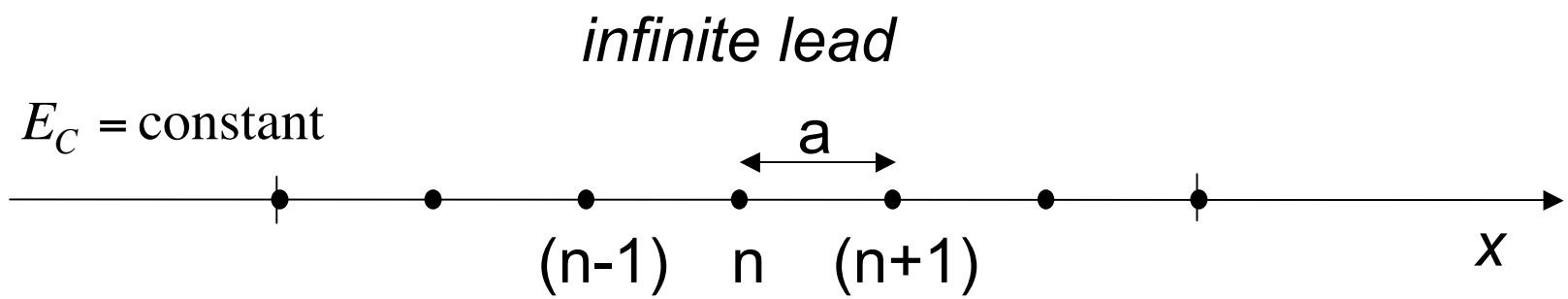
$$E - E_C = \hbar^2 k^2 / 2m^*$$

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

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

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

II) Solving the Wave Equation: E_k in the leads



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

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

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

II) Solving the Wave Equation: E_k in the leads

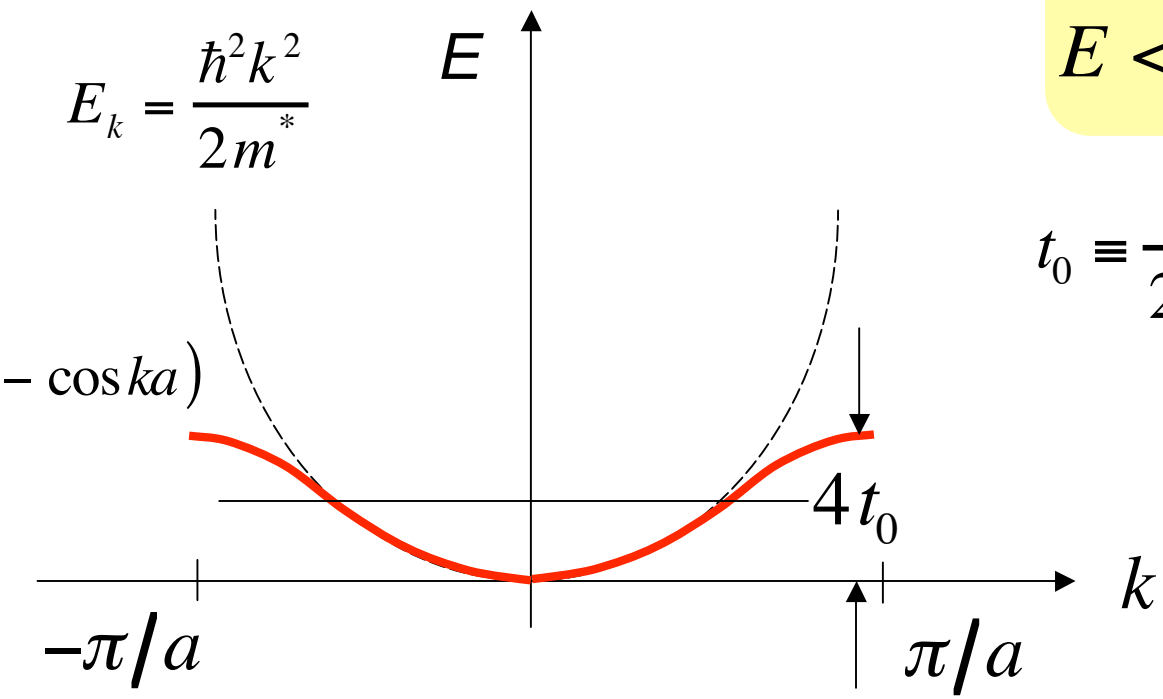
be sure!

$$E << 4t_0$$

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

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

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



1) Introduction
2) Solving the Wave Equation
3) **Computing n(x)**
4) Computing I_D
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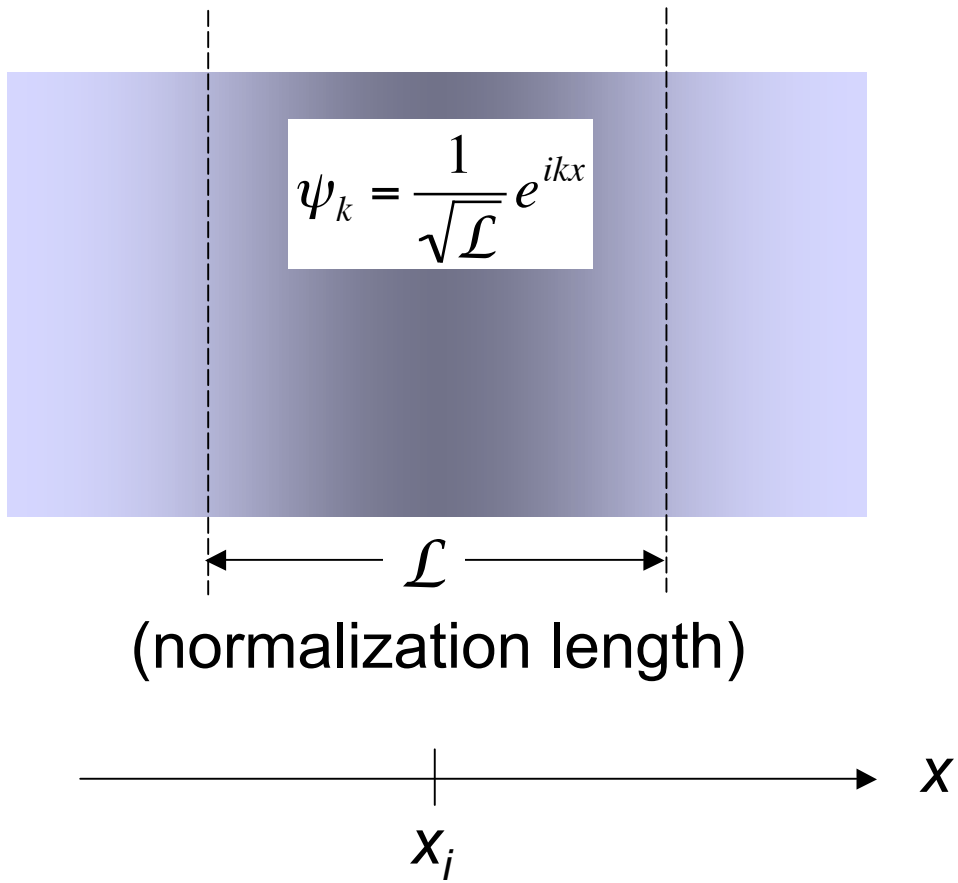
III) Computing n(x): in the bulk

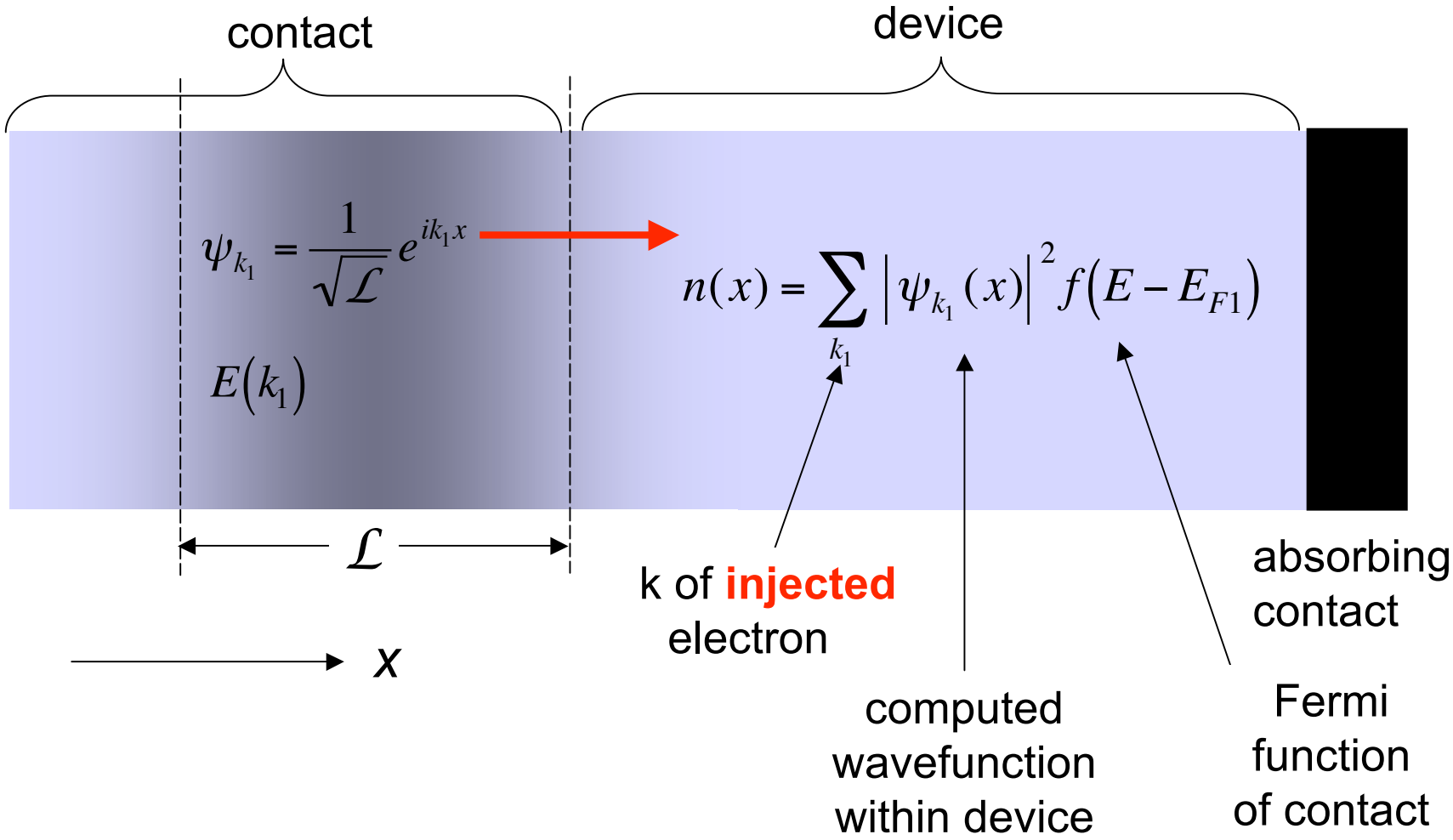


$$n(x_i) = \sum_k \left|\psi_k(x_i)\right|^2 f\left(E - E_F\right)$$

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

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

$$n_1(x_i) = \frac{1}{\mathcal{L}} \sum_{k_1} \left| \psi_{k_1}(x_i) \right|^2 f\left(E - E_{F1}\right)$$

normalization length in the **contact**

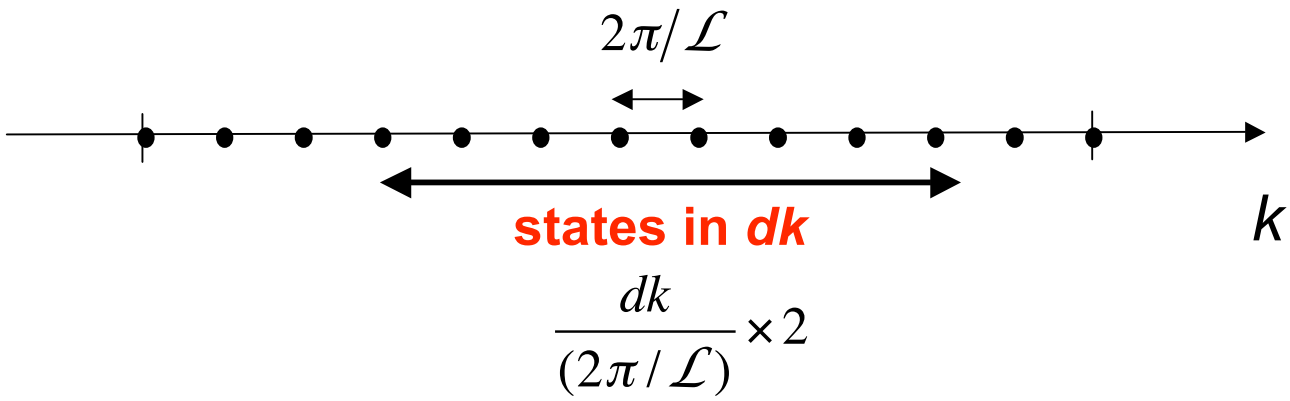
$$\psi_{k_1} = \frac{1}{\sqrt{\mathcal{L}}} e^{ik_1 x}$$

computed assuming unit amplitude injected wave

weight by Fermi function of the source

III) Computing n(x)

$$n_1(x_i) = \frac{1}{\mathcal{L}} \sum_{k_1 > 0} \left| \psi_{k_1}(x_i) \right|^2 f\left(E - E_{F1}\right)$$



$$n_1(x_i) = \frac{1}{\mathcal{L}} \frac{\mathcal{L}}{2\pi} \times 2 \int_0^\infty dE \frac{dk_1}{dE} \left| \psi_{k_1}(x_i) \right|^2 f\left(E - E_{F1}\right)$$

III) Computing n(x)

$$n_1(x_i) = \underbrace{\int_0^{\infty} \left[\frac{1}{\pi} \frac{dk_1}{dE} \left| \psi_{k_1}(x_i) \right|^2 \right]}_{LDOS_1(x_i, E)} f_0\left(E - E_{F1}\right) dE$$

this is the **portion** of the local density-of-states within the device due to **injection from contact 1**.

III) Computing n(x)

$$n(x_i) = \int_0^\infty LDOS_1(x_i,E) f_0\left(E - E_{F1}\right) dE + \int_0^\infty LDOS_2(x_i,E) f_0\left(E - E_{F2}\right) dE$$

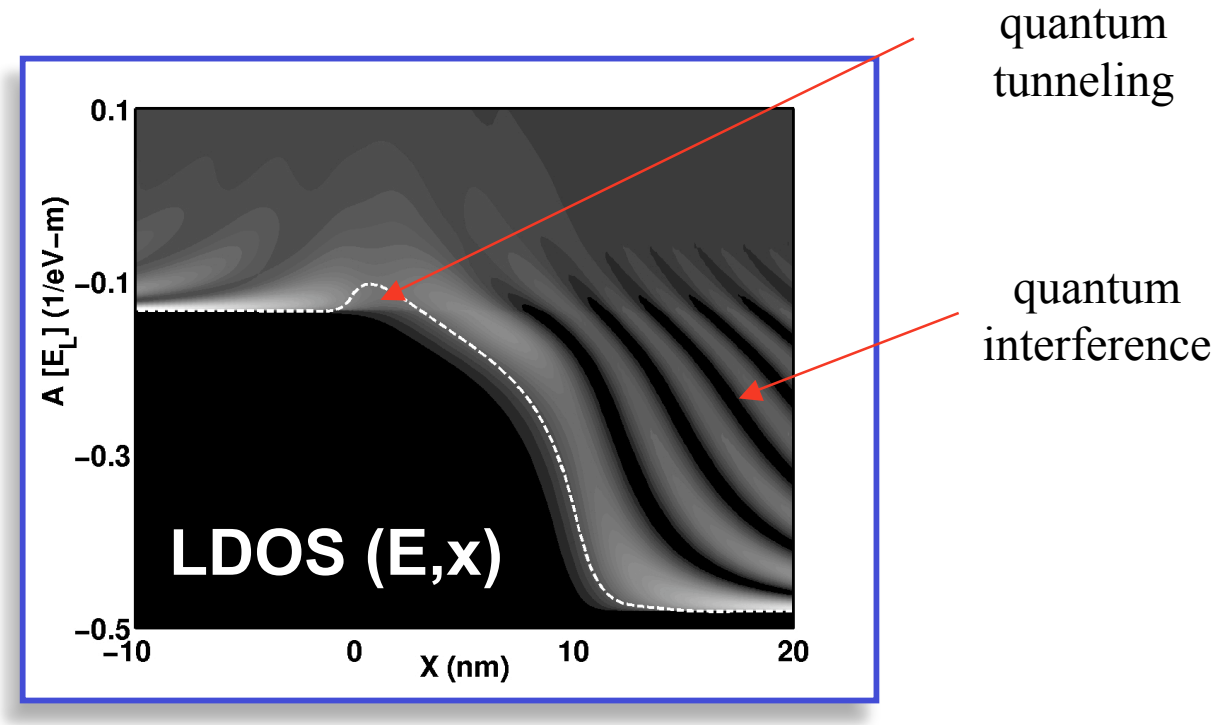
LDOS$_1$, *LDOS*$_2$ can be computed semi-classically

or

quantum mechanically

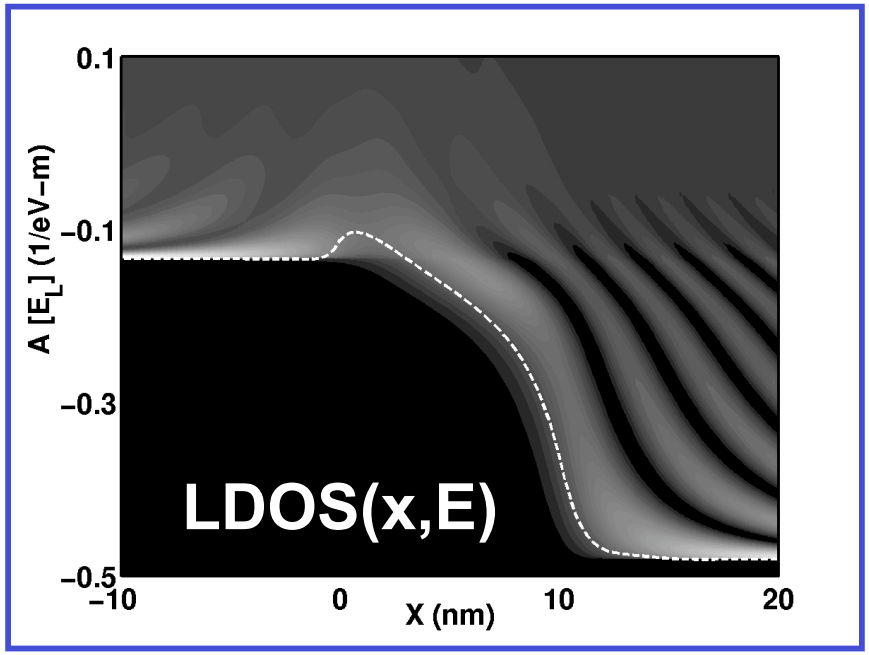
III) Computing n(x): local DOS in a MOSFET

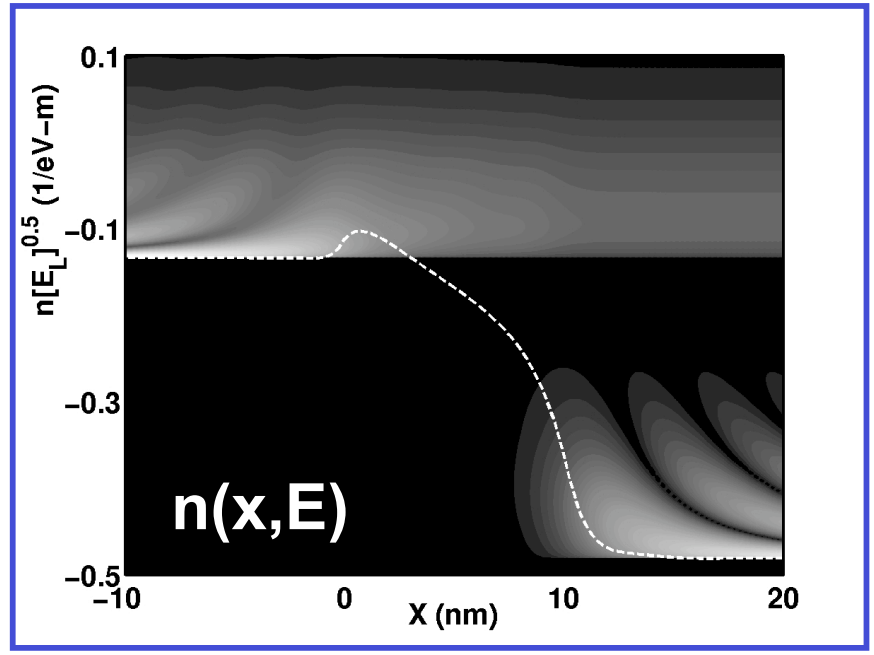
$$LDOS_1(x_i,E) = \left[\frac{1}{\pi}\frac{dk_1}{dE}\left|\psi_{k_1}(x_i)\right|^2\right] \qquad LDOS_2(x_i,E) = \left[\frac{1}{\pi}\frac{dk_2}{dE}\left|\psi_{k_2}(x_i)\right|^2\right]$$



III) Computing n(x)

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



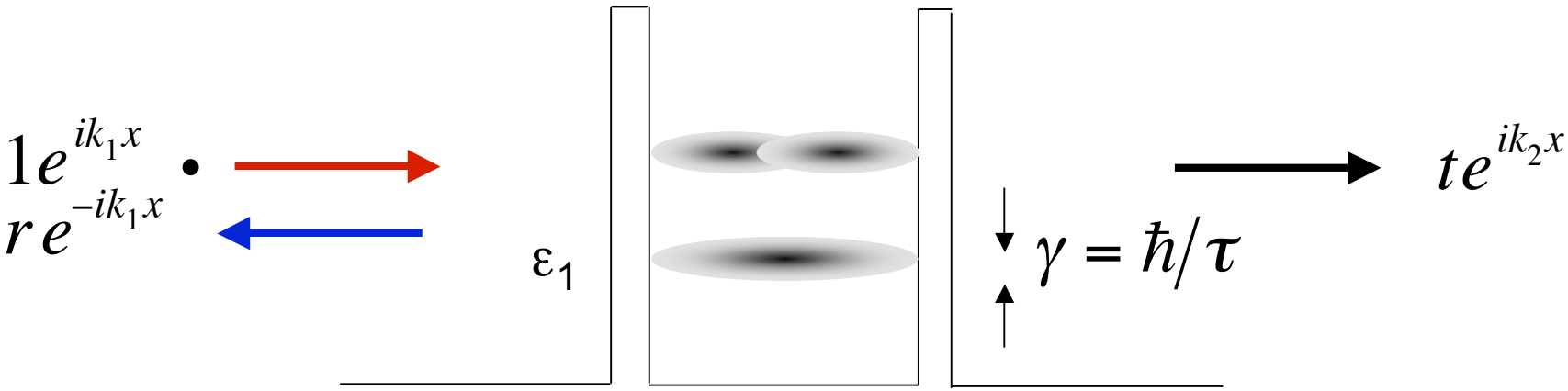


$$LDOS(x,E) = LDOS_1(x,E) + LDOS_1(x,E)$$

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

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

III) Computing n(x): bound states again



"broadening"

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IV) Computing I_D

let's derive the current expression beginning with:

$$I_{1-2} = \frac{q}{\mathcal{L}} \sum_{k_1 > 0} T_{1-2}(E) \upsilon_{k_1} \; f(E - E_{F1})$$

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

$$I_{1-2} = \frac{q}{\pi} \int T_{1-2}(E) \upsilon_{k_1} f(E - E_{F1}) dk_1$$

IV) Computing I_D

$$I_{1-2} = \frac{q}{\pi} \int_{k_1 > 0} T_{1-2}(E) \upsilon_{k_1} f(E - E_{F1}) dk_1$$

$$= \frac{q}{\pi \hbar} \int_{k > 0} T_{1-2}(E) \frac{dE}{d(\hbar k)} f(E - E_{F1}) dk$$

$$I_{1-2} = \frac{2q}{h} \int_{0} T_{1-2}(E) f(E - E_{F1}) dE$$

IV) Computing I_D

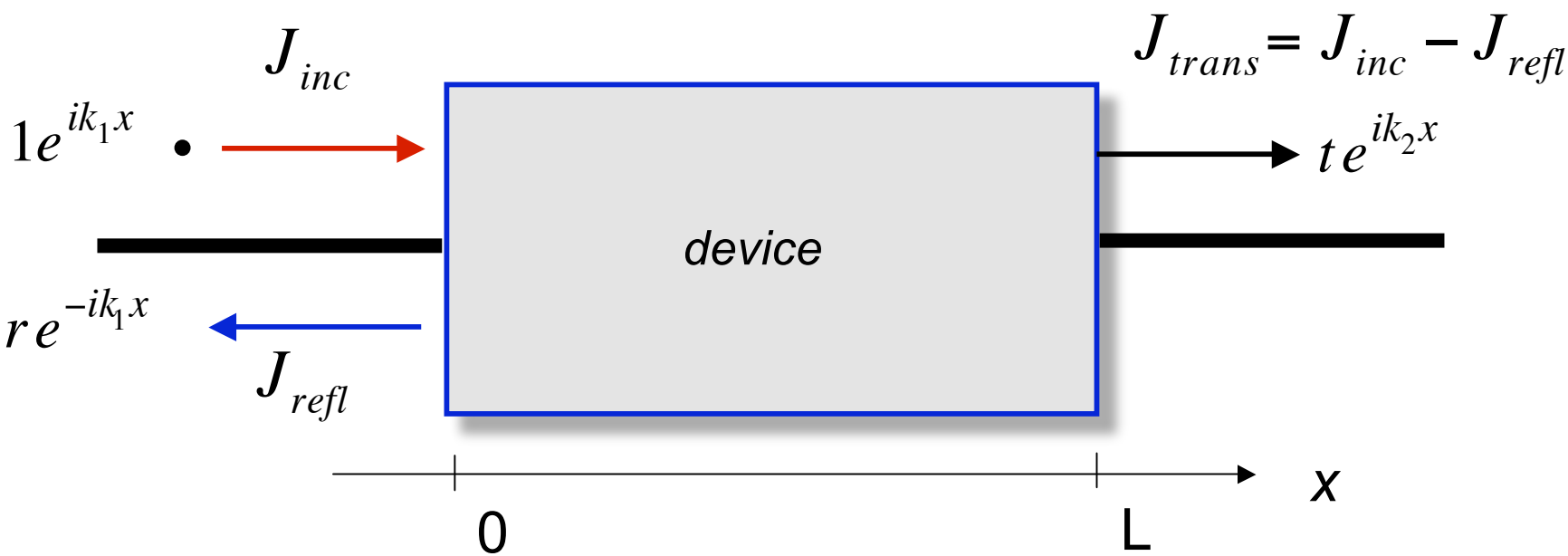
$$I_D = I_{1-2} - I_{2-1}$$

$$\left.\begin{aligned} I_{1-2} &= \frac{2q}{h}\int_0 T_{1-2}(E)\, f(E - E_{F1})\, dE \\ I_{2-1} &= \frac{2q}{h}\int_0 T_{2-1}(E)\, f(E - E_{F2})\, dE \end{aligned}\right\} \quad T_{1-2}(E) = T_{2-1}(E)$$

(ballistic)

$$I_D = \frac{2q}{h}\int_0 T(E)\left[f(E - E_{F1}) - f(E - E_{F2})\right] dE$$

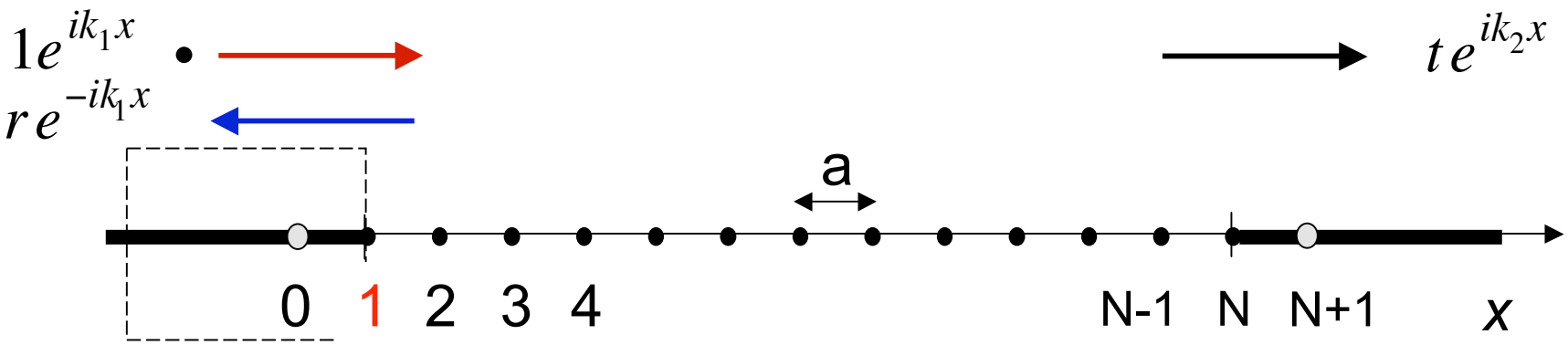
IV) Computing I_D: Finding $T_{1\text{-}2}(E)$



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

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

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



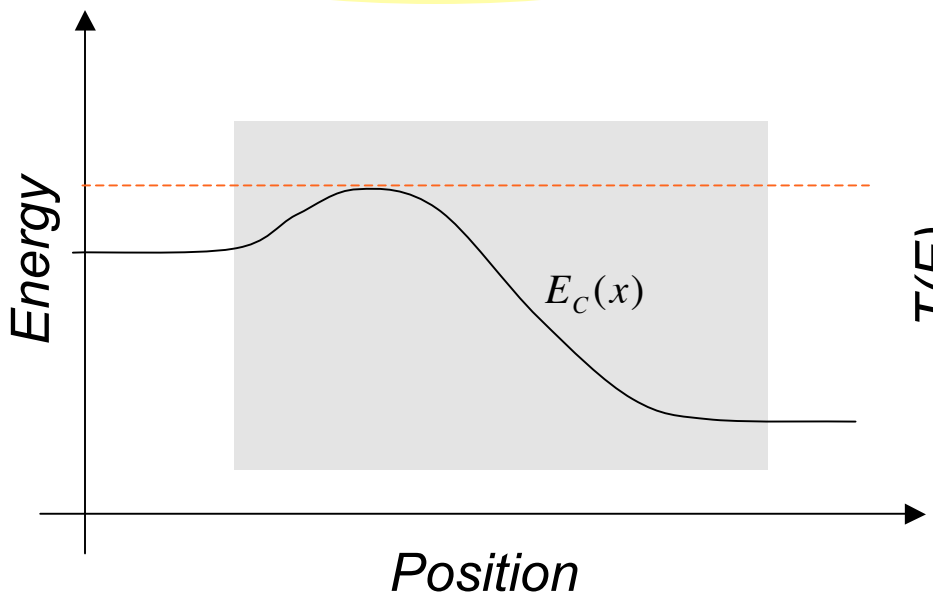
$$\psi(x) = 1e^{ik_1x} + re^{-ik_1x} \qquad x \le 0$$

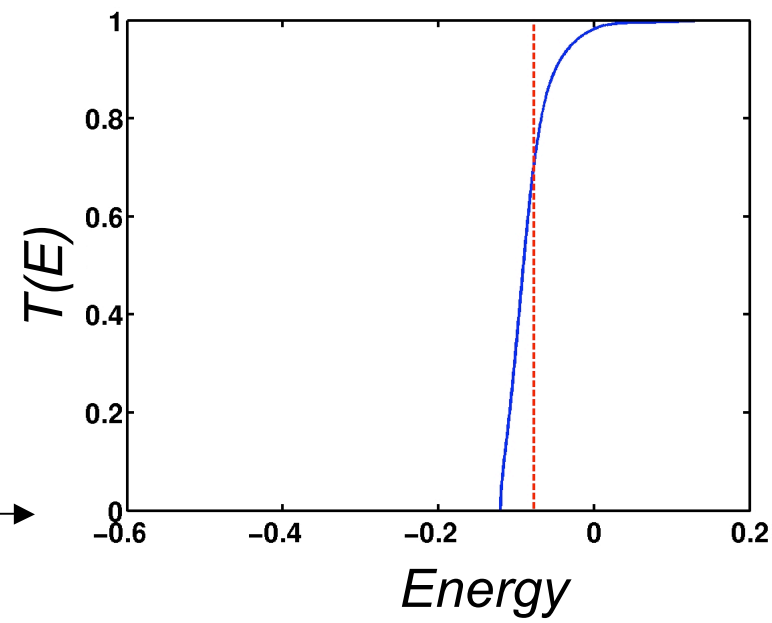
$$\psi(x=0) = 1 + r = \psi_1$$

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

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

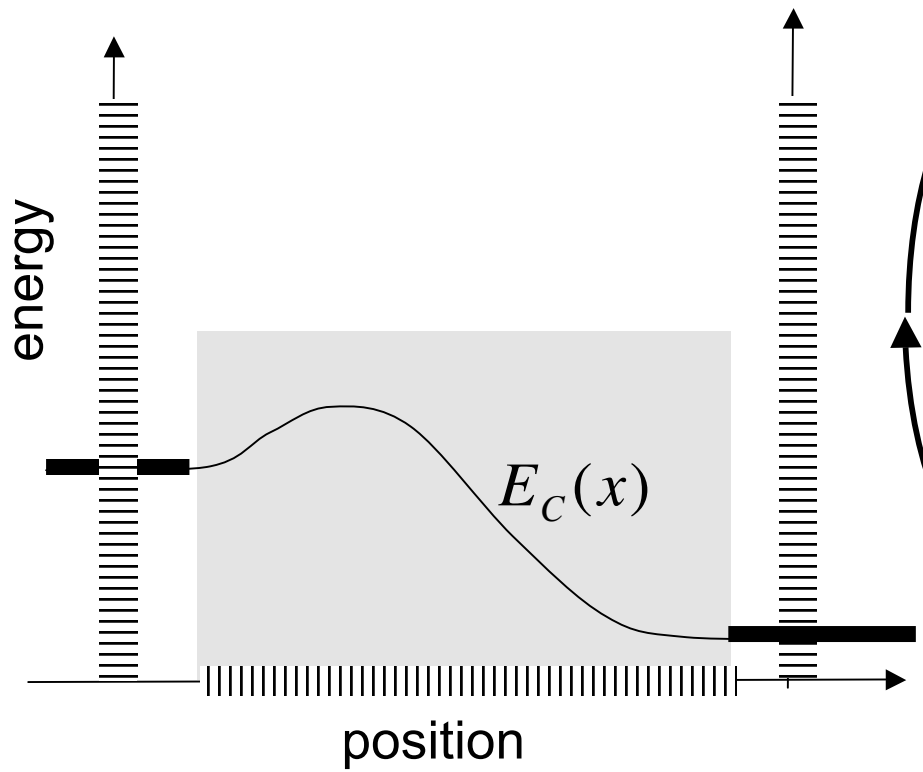
$$T_{1-2}(E) = 1 - \left|\psi_1 - 1\right|^2$$





1) Introduction
2) Solving the Wave Equation
3) Computing n(x)
4) Computing I_D
5) **NEGF Formulation**
6) Scattering
7) Summary

V) NEGF Formulation: 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 2

6) Determine I_D

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

energy channels are independent!
(ballistic)

V) NEGF Formulation: Key Results

$$\left[E\mathbf{I} - \mathbf{H} - \sum_1 - \sum_2\right]_{\mathrm{NxN}} \boldsymbol{\psi}_{\mathrm{Nx1}} = i\,\boldsymbol{\gamma}_{\mathrm{Nx1}}$$

$$n_1(x_i) = \int_0^{E_{Top}} LDOS_1(x_i, E) f\left(E - E_{F1}\right) dE$$

$$LDOS_1\left(x_i, E\right) = 2 \times \left(\frac{1}{2\pi}\frac{dk}{dE}\left|\psi_k(x_i)\right|^2\right)$$

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

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

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

$$\mathbf{G}_{\mathrm{NxN}} = \left[E\mathbf{I} - \mathbf{H} - \sum_{\mathbf{1}} - \sum_{\mathbf{2}}\right]^{-1}_{\mathrm{NxN}}$$

Can we do everything with the Green's function?

V) NEGF Formulation: density matrix

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

We have:

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

V) NEGF Formulation: density matrix

(N x 1) $$n_1(x_i) = \int_0^{E_{Top}} 2 \times \frac{1}{2\pi} \frac{dk}{dE} \left| \psi_k(x_i) \right|^2 f\left(E - E_{F1}\right) dE$$

$$\left| \psi_k(x_i) \right|^2 \rightarrow \mathbf{G} \boldsymbol{\gamma} \boldsymbol{\gamma}^H \mathbf{G}^H$$

(N x N) $$\rho_1 = \int_0^{E_{Top}} \frac{1}{\pi} \frac{dk}{dE_k} \left\{ \mathbf{G} \boldsymbol{\gamma}_1 \boldsymbol{\gamma}_1^{\mathbf{H}} \mathbf{G}^{\mathbf{H}} \right\} f\left(E - E_{F1}\right) dE$$

V) NEGF Formulation: 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) NEGF Formulation: density matrix

$$\rho_1 = \int_0^{E_{Top}} 2 \times \frac{1}{2\pi} \frac{dk}{dE} \left\{ \mathbf{G} \gamma_1 \gamma_1^{\mathbf{H}} \mathbf{G}^{\mathbf{H}} \right\} f\left(E - E_{F1}\right) dE$$

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

$$\frac{dk}{dE} = \frac{1}{2a t_0 \sin ka}$$

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

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

V) NEGF Formulation: spectral function

$$\rho_1 = \int_0^{E_{Top}} 2 \times \frac{1}{2\pi} \frac{dk}{dE} \left\{ \mathbf{G} \boldsymbol{\gamma}_1 \boldsymbol{\gamma}_1^{\mathbf{H}} \mathbf{G}^{\mathbf{H}} \right\} f\left(E - E_{F1}\right) dE$$

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

$$\rho_1 \Big|_{\mathrm{NxN}} = \int 2 \times \frac{\mathbf{A_1}\big|_{\mathrm{NxN}}}{2\pi} f\left(E - E_{F1}\right) dE$$

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

V) NEGF Formulation: recap

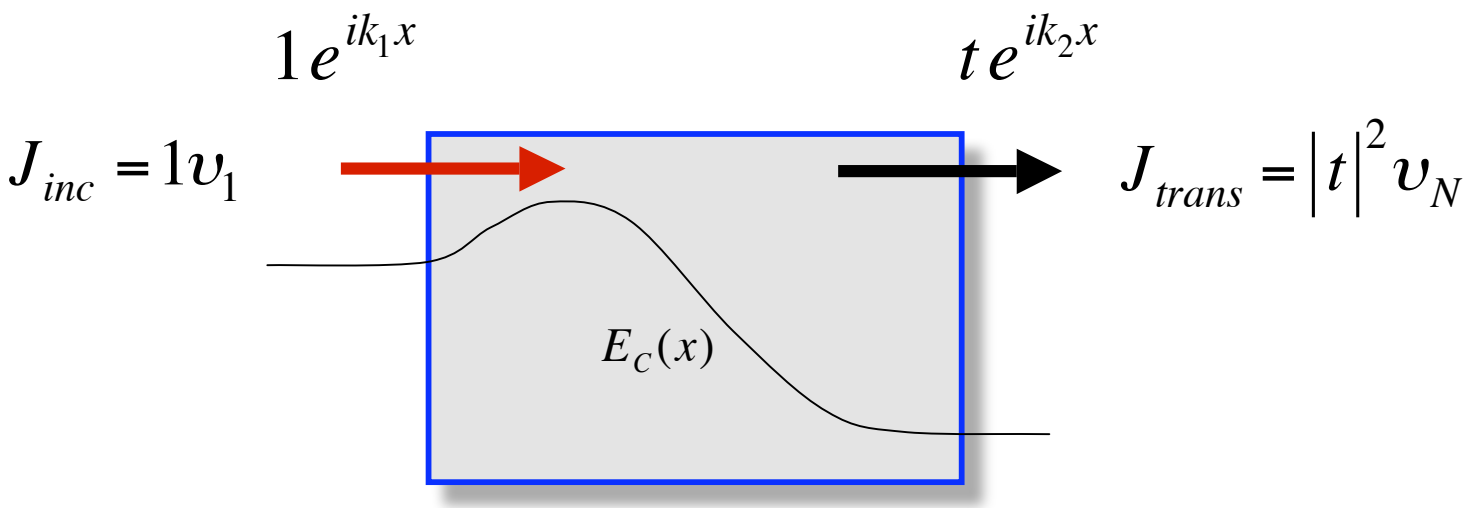
1) $\mathbf{G} = \left[E\mathbf{I} - \mathbf{H} - \sum_{\mathbf{1}} - \sum_{\mathbf{2}} \right]^{-1}$ (retarded Green's function)

2) $\mathbf{\Gamma}_1 = i\left(\mathbf{\Sigma}_1 - \mathbf{\Sigma}_1^H \right)$ (broadening)

3) $\mathbf{A_1} = \mathbf{G}\,\mathbf{\Gamma}_1 \mathbf{G}^{\mathbf{H}}$ (spectral function)

4) $\rho_1 \Big|_{\mathrm{NxN}} = \int 2 \times \frac{\mathbf{A_1}\big|_{\mathrm{NxN}}}{2\pi} f\left(E - E_{F1}\right) dE$ (density matrix)

V) NEGF Formulation: transmission



$$T_{1-2} = |t|^2 \left(\frac{\upsilon_N}{\upsilon_1} \right)$$

V) NEGF Formulation: transmission

$$T^{1-2} = |t|^2 \left(\frac{\upsilon_N}{\upsilon_1} \right)$$

$$|t|^2 = |\psi_N|^2$$

$$\psi_N = G(N,1)\Gamma_1(1,1)$$

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

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

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

$$T^{1-2}(E) = \mathrm{trace}\left[\Gamma_1 \mathbf{G} \Gamma_2 \mathbf{G}^{\mathrm{H}}\right]$$

V) NEGF Formulation: key results in NEGF form

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

$$\rho_1 = \int 2 \times \frac{dE}{2\pi} \mathbf{A}_1(E) f\left(E_F - E\right)$$

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

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

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

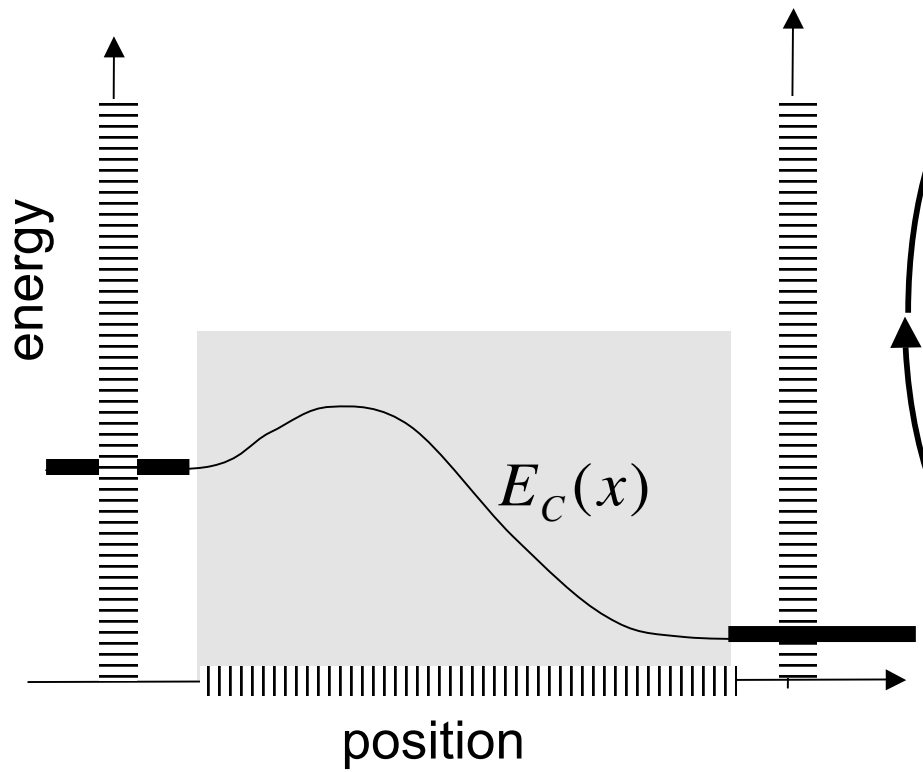
$$\mathbf{\Sigma}_1 = \begin{bmatrix} -t_0 e^{ik_1 a} & 0 & \dots \\ 0 & 0 & \dots \\ \dots & \dots & \dots \end{bmatrix}$$

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

$$\mathbf{\Gamma}_1 = i\left[\mathbf{\Sigma}_1 - \mathbf{\Sigma}_1^H\right]$$

$$\mathbf{\Gamma}_2 = i\left[\mathbf{\Sigma}_2 - \mathbf{\Sigma}_2^H\right]$$

V) NEGF Formulation: key results in NEGF form



1) Guess $U_{SCF}(x)$
2) For each energy:

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

3) Determine $\rho(x)$:

$$\rho = \int 2 \times \frac{\mathbf{A}(E)}{2\pi} f\left(E - E_{F1}\right) dE$$

4) solve Poisson for $U_{SCF}(x)$
5) go to 2

6) Determine I_D from $T(E)$

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

energy channels are independent!
(ballistic)

1) Introduction
2) Solving the Wave Equation
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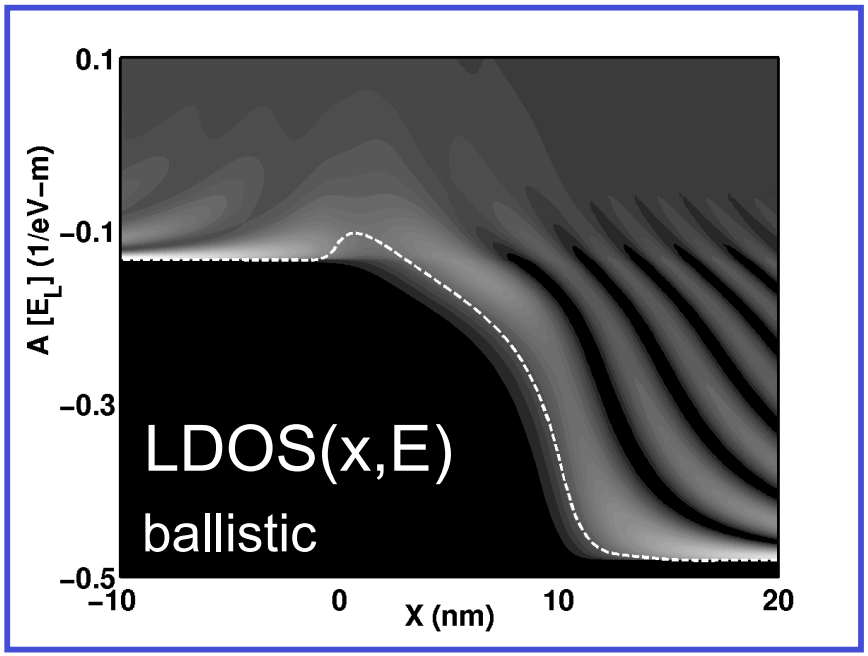
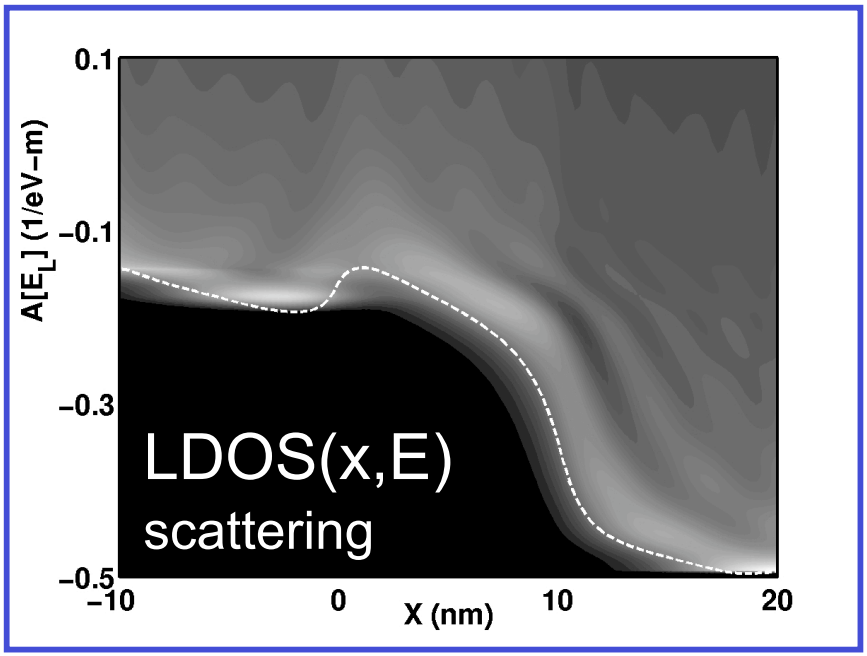
4) Computing I_D
5) NEGF Formulation
6) **Scattering**
7) Summary

VI) Scattering

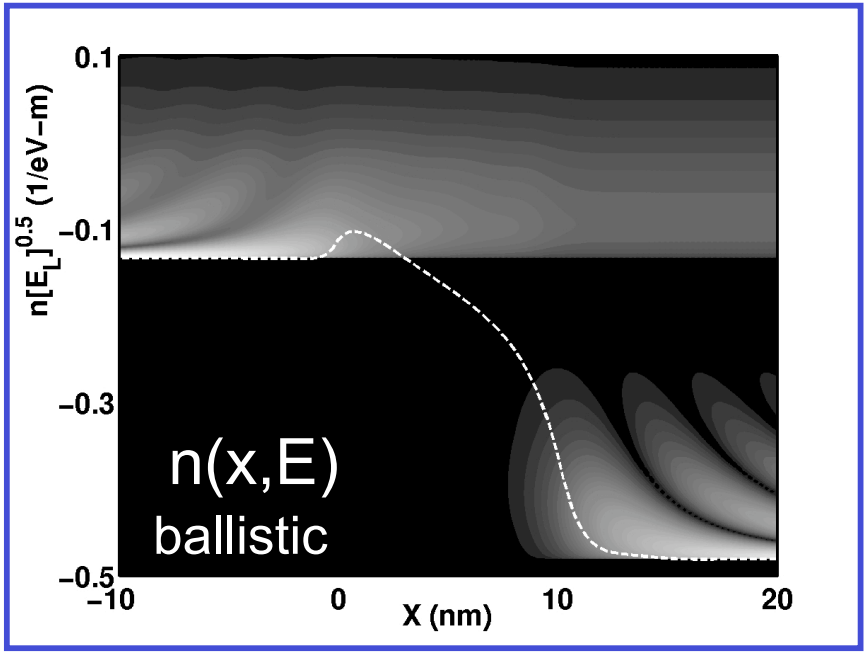
(on-state, V_{DD} = 0.4 V)

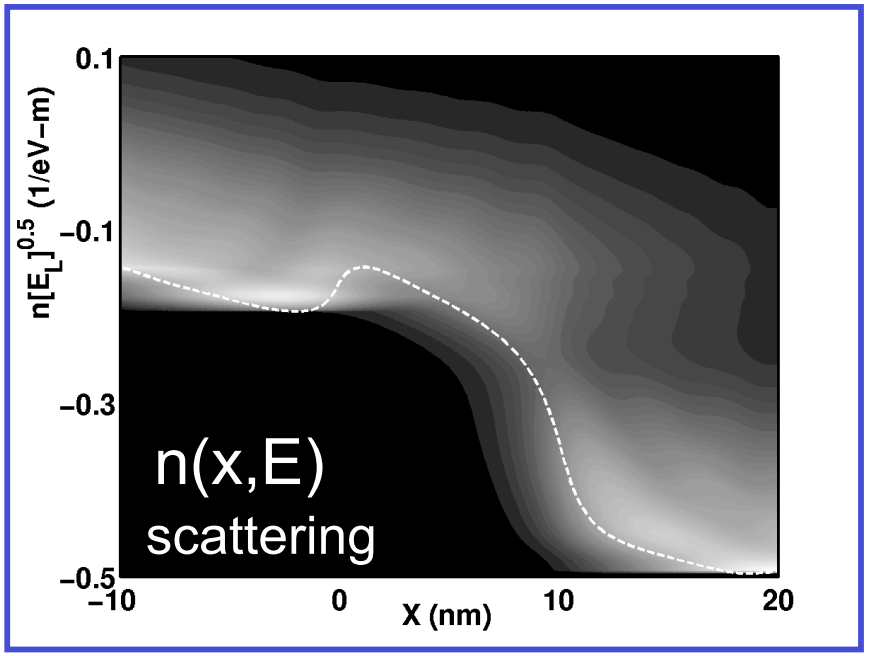




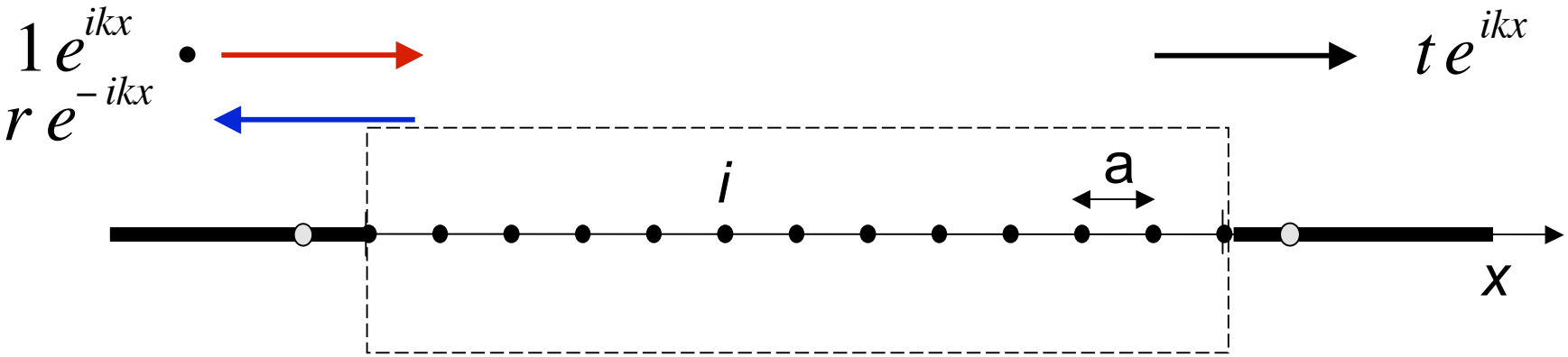
VI) Scattering

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





VI) Scattering: filling states from contacts”



$$\mathbf{G}(E) = \left[\mathbf{EI} - \mathbf{H} - \mathbf{\Sigma}_1 - \mathbf{\Sigma}_2\right]^{-1}$$

$$\mathbf{G}^n(E) = f_1(E)\mathbf{A}_1(E) + f_2(E)\mathbf{A}_2(E)$$

$$\rho = 2 \times \int dE \frac{\mathbf{G}^n(E)}{2\pi}$$

VI) Scattering: "in- and out-scattering from contacts"

$$\mathbf{G}^n(E) = f_1\mathbf{A}_1(E) + f_2\mathbf{A}_2(E) = \mathbf{G}\,\Sigma_1^{in}\,\mathbf{G}^H + \mathbf{G}\,\Sigma_2^{in}\,\mathbf{G}^H$$

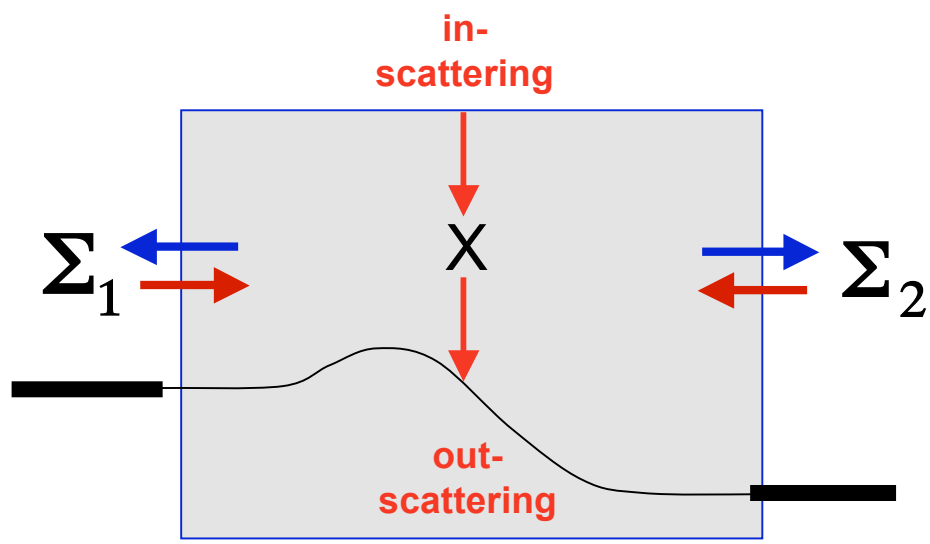
$$\left[\Sigma_{1,2}^{in} = f_{1,2}\Gamma_{1,2}\right]$$ "in-scattering"

$$\mathbf{G}^p(E) = \left(1 - f_1\right)\mathbf{A}_1(E) + \left(1 - f_2\right)\mathbf{A}_2(E) = \mathbf{G}\,\Sigma_1^{out}\,\mathbf{G}^H + \mathbf{G}\,\Sigma_2^{out}\,\mathbf{G}^H$$

$$\left[\Sigma_{1,2}^{out} = \left(1 - f_{1,2}\right)\Gamma_{1,2}\right]$$ "out-scattering"

$$\left[\Sigma_{1,2}^{in} + \Sigma_{1,2}^{out} = \Gamma_{1,2}\right]$$

VI) Scattering

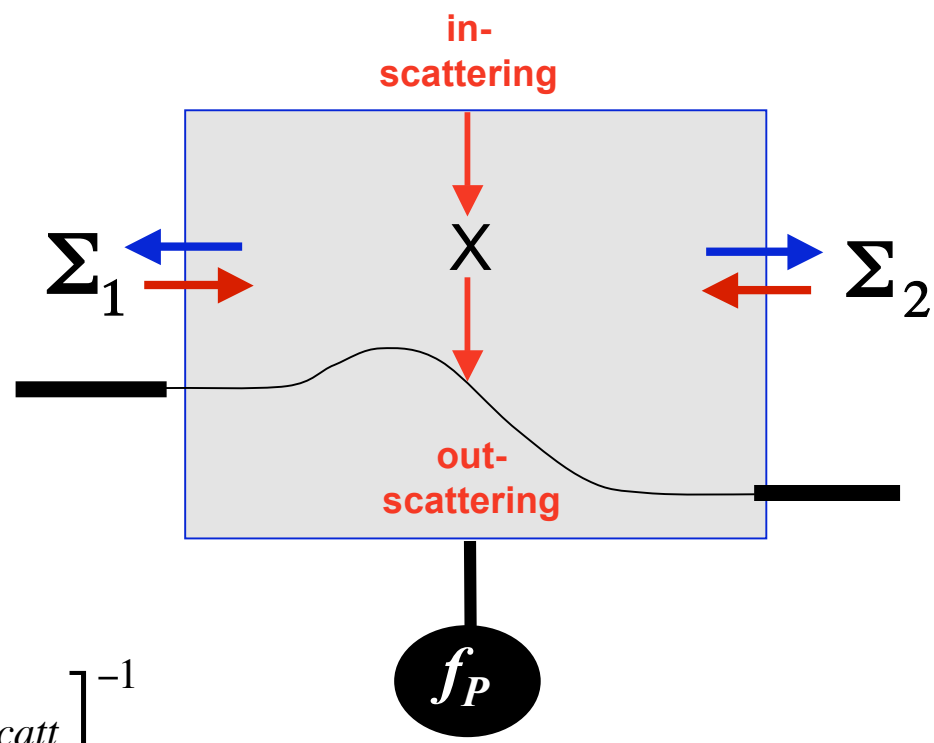


$$\mathbf{G}(E) = \left[\mathbf{EI} - \mathbf{H} - \mathbf{\Sigma}_1 - \mathbf{\Sigma}_2 - \mathbf{\Sigma}_{Scatt}\right]^{-1}$$

$$\mathbf{G}^n(E) = \mathbf{G} f_1 \Gamma_1 \mathbf{G}^H + \mathbf{G} f_2 \Gamma_2 \mathbf{G}^H + \mathbf{G} \Sigma_{Scatt}^{in} \mathbf{G}^H$$

VI) Scattering: Buttiker probes

$$\Sigma_{Scatt} = \begin{bmatrix} 0 & 0 & \dots \\ 0 & t_S e^{ika} & 0 \\ \dots & 0 & 0 \end{bmatrix}_{N \times N}$$



$$\mathbf{G}(E) = \left[\mathbf{EI} - \mathbf{H} - \mathbf{\Sigma}_1 - \mathbf{\Sigma}_2 - \mathbf{\Sigma}_{Scatt} \right]^{-1}$$

$$\mathbf{G}^n(E) = \mathbf{G} f_1 \Gamma_1 \mathbf{G}^H + \mathbf{G} f_2 \Gamma_2 \mathbf{G}^H + \mathbf{G} \Sigma_{Scatt}^{in} \mathbf{G}^H$$

$$\mathbf{\Sigma}_{Scatt}^{in} = f_P \mathbf{\Gamma}_{Scatt} = f_P \, i \left(\mathbf{\Sigma}_{Scatt} - \mathbf{\Sigma}_{Scatt}^H \right)$$

VI) Scattering: Fermi's Golden Rule

$$\mathbf{G}(E) = \left[\mathbf{EI} - \mathbf{H} - \mathbf{\Sigma}_1 - \mathbf{\Sigma}_2 - \mathbf{\Sigma}_{Scatt}\right]^{-1}$$

$$\mathbf{G}^n(E) = \mathbf{G}\Sigma^{in}\mathbf{G}^H \qquad \left(\Sigma^{in} = \Sigma_1^{in} + \Sigma_2^{in} + \Sigma_{Scatt}^{in}\right)$$

$$\Sigma_{Scatt}$$

$$\mathbf{\Sigma}_{Scatt}^{in}(E) \propto G^n(E \pm \hbar\omega)\Gamma_{Scatt} \qquad \left(\Gamma_{Scatt} = i\left[\Sigma_{Scatt} - \Sigma_{Scatt}^H\right]\right)$$

see: Chapter 8 in S. Datta, *Electronic Transport in Mesoscopic Systems*, Cambridge Univ. Press, 1995.

VII) Summary

1) Boltzmann Transport Equation

$$f\left(r,k\right)$$

2) Non-equilibrium Green's function formalism

$$\mathbf{G}\left(r,r',E\right)$$

1) The NEGF provides a convenient formalism for solving the single particle Schrödinger equation with open boundary conditions.
2) NEGF can describe devices at a continuum (eff mass) or atomistic (e.g. tight binding) level.
3) NEGF also provides a rigorous basis for going beyond the single electron Schrödinger equation.
4) NEGF is rapidly becoming an essential tool for device engineers.

References

1) Supriyo Datta, “nanoscale Device Modeling: The Green’s Function Method,” *Superlattices and Microsctructures*, **28**, 253, 2000.

2) Supriyo Datta, “Electrical Resistance: an atomistic view,” *Nanotechnology*, **15**, S433-S451, 2004.

3) Supriyo Datta, *Electronic Transport in Mesoscopic Systems*, Cambridge Univ. Press, 1995

4) Roger lake, gerhard Klimeck, Chris Bowen, and Dejan Jovanovic, “Single and Multiband Modeling of Quantum Electron Transport Through layered Semiconductor Devices,” J. Appl. Phys., 81, 7845, 1997.

5) Ph.D. theses of Zhibin Ren, Ramesh Venugopal, and Jing Guo, available at http://ece.purdue.edu/~lundstro

6) **www.nanohub.org**