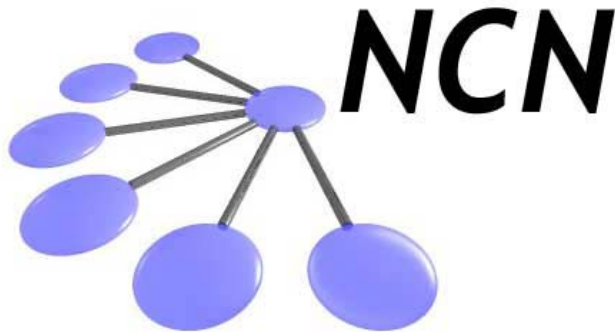


Network for Computational Nanotechnology (NCN)

US Berkeley, Univ. of Illinois, Norfolk State, Northwestern, Purdue, UTEP

NEGF in a Quasi-1D formulation

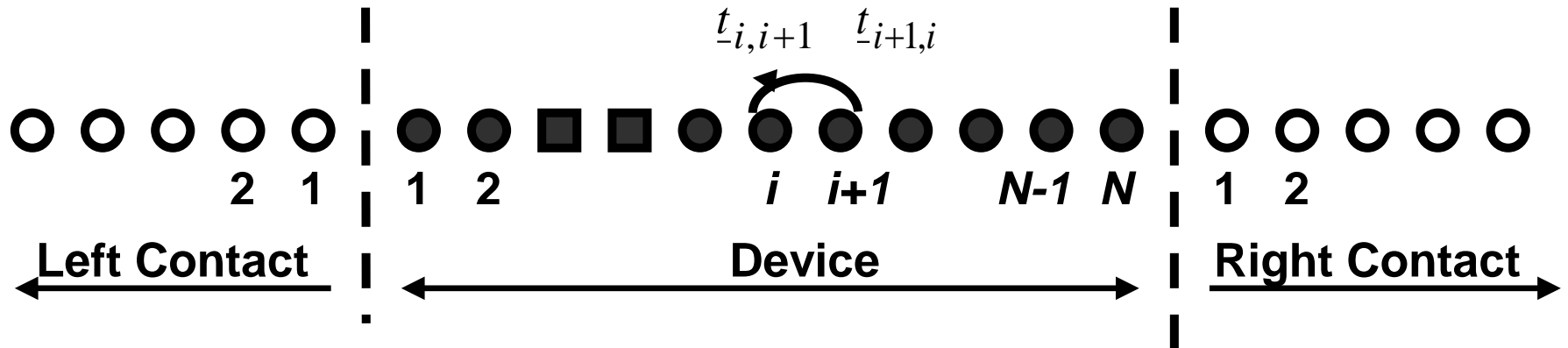
Gerhard Klimeck,
Samarth Agarwal, Zhengping Jiang



NEGF in a Quasi-1D formulation

- Effective Mass Tight-Binding Hamiltonian in 1D discretized Schrödinger Eq.
- Quantum Transmitting Boundary Method (QTBM)
Open Boundary Conditions
- Fundamental NEGF Equations

Partitioning of the simulation domain into three regions



- Left contact with index L, the central device region with index D and right contact with index R.
- In central device, one solves the non-equilibrium transport equations.
- Contacts are assumed to be in local equilibrium.

Build difference effective-mass Schrodinger's equation

- Recall: 1D effective-mass Schrodinger's equation \rightarrow differential equation

$$E\psi = -\frac{\hbar^2}{2} \frac{\delta}{\delta x} \frac{1}{m^*(x)} \frac{\delta}{\delta x} \psi + V(x)\psi$$

- finite-difference approximation $\rightarrow x_j = j\Delta$
 - » assume: effective-mass did not vary $\rightarrow m^*(x) = m^*$
 - » Three points approximation for second derivative:

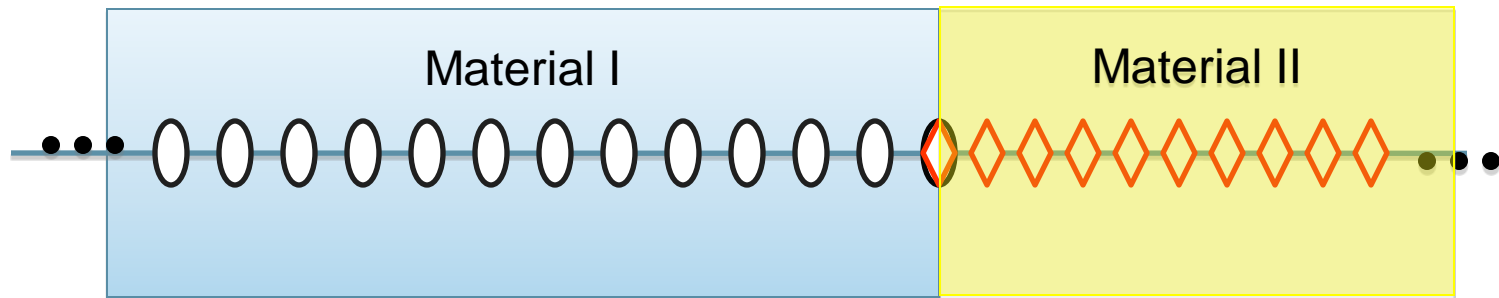
$$\frac{\partial^2 \psi}{\partial x^2} \approx \frac{\psi(x-\Delta) - 2\psi(x) + \psi(x+\Delta)}{\Delta^2}$$

$$H\psi_j = -s_j\psi_{j-1} + d_j\psi_j - s_{j+1}\psi_{j+1} = E\psi_j \rightarrow \text{difference form}$$

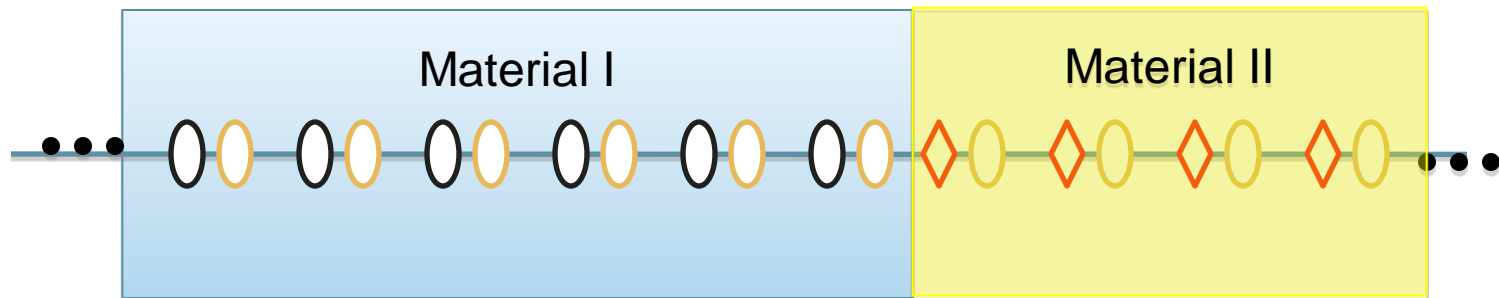
- If $m^*(x)$ is allowed to vary... which is real in heterostructure
 - » Variation will be included in values of s_j, d_j (continued...)

Schemes of mesh discretization

- Continuum thinking - Put mesh points at the interfaces.
 - » Some problems in the interface...(next slide)



- Atomistic thinking: place meshpoints at positions of atoms:
A-B atoms mesh: real device → Ga-As-Ga-As-Al-As-Al-As.
 - » Interface is between atoms!



Mapping effective mass to mesh points

- Simple fashion
 - » Recall: we use a discrete mesh
 - » wavefunction vary linearly between ψ_j and ψ_{j+1}
 - » m^* constant across interval j to $j+1$
 - equation set 1
- Problem: heterostructure on a mesh point
 - » make heterostructure between two adjacent mesh points
 - equation set 2
- Considering matching condition on wavefunction
 - » ψ and its first derivative must be continuous in heterostructure
 - » derive from 1 and 2, apply matching condition
 - equation set 3 (final)

$$d_j = \frac{\hbar^2}{2\Delta^2} \left(\frac{1}{m_{j-\frac{1}{2}}^*} + \frac{1}{m_{j+\frac{1}{2}}^*} \right) + V_j$$

$$s_j = \frac{\hbar^2}{2\Delta^2 m_{j+\frac{1}{2}}^*} \quad \mathbf{1}$$

$$d_j = \frac{\hbar^2}{4\Delta^2} \left(\frac{1}{m_{j-1}^*} + \frac{2}{m_j^*} + \frac{1}{m_{j+1}^*} \right) + V_j$$

$$s_j = \frac{\hbar^2}{4\Delta^2} \left(\frac{1}{m_{j-1}^*} + \frac{1}{m_j^*} \right) \quad \mathbf{2}$$

$$d_j = \frac{\hbar^2}{\Delta^2} \left(\frac{1}{m_{j-1}^* + m_j^*} + \frac{1}{m_j^* + m_{j+1}^*} \right) + V_j$$

$$s_j = \frac{\hbar^2}{\Delta^2} \frac{1}{m_{j-1}^* + m_j^*} \quad \mathbf{3}$$

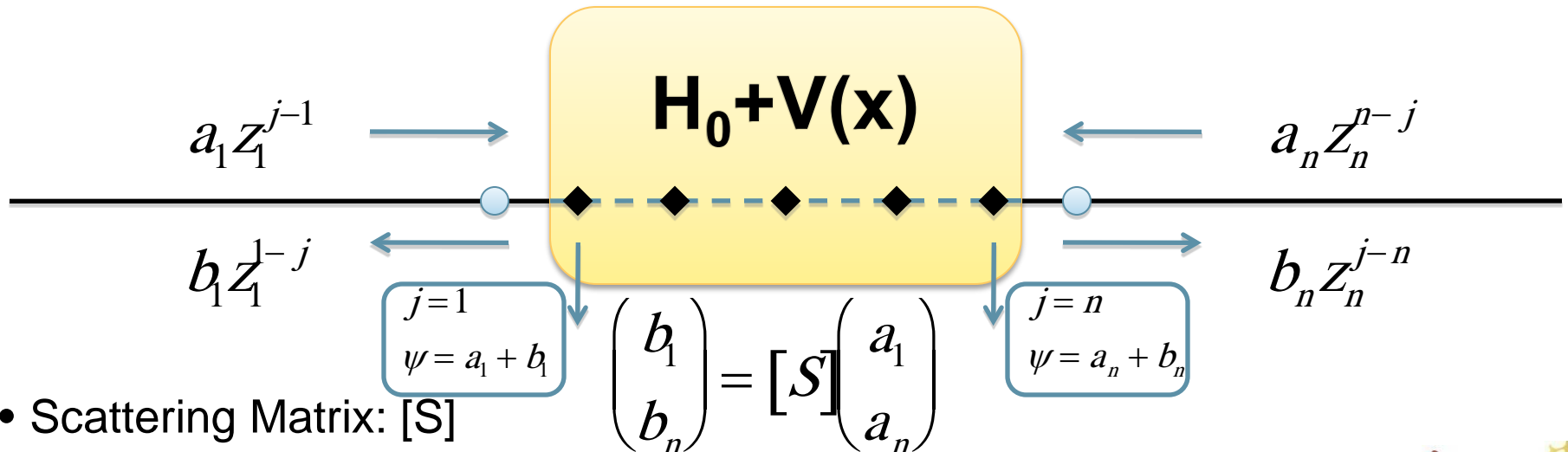
Quantum Transmitting Boundary Method (QTBM) in discrete case

- Contact: semi-infinite, potential vary smoothly
- $j=1$ and $j=n \rightarrow$ limits of domain where potential vary
 - » boundary points: $j=0$ and $j=n+1$

$$j \leq 1 \dots \dots \psi_j = a_1 z_1^{j-1} + b_1 z_1^{1-j}$$

$$j \geq n \dots \dots \psi_j = a_n z_n^{n-j} + b_n z_n^{j-n}$$

- » propagating states $z = e^{ik\Delta}$
- » evanescent states $z = e^{-\gamma\Delta}$



- Scattering Matrix: $[S]$

Quantum Transmitting Boundary Method (QTBM) in discrete case

- To get z , substitute to difference equation:

» solve for z , z_n :

$$E = d_1 - s_1 (z_1 + z_1^{-1})$$

$$E = d_n - s_n (z_n + z_n^{-1})$$

- For the boundary points: →

$$\psi_0 = a_1 z_1^{-1} + b_1 z_1$$

$$\psi_1 = a_1 + b_1$$

$$\psi_n = a_n + b_n$$

$$\psi_{n+1} = a_n z_n^{-1} + b_n z_n$$

- To obtain QTBM equation

» Solve for a_1 , a_n , add to matrix →

$$a_1 = \frac{\psi_0 - z_1 \psi_1}{z_1^{-1} - z_1} = \alpha_1 \psi_0 + \beta_1 \psi_1$$

$$a_n = \frac{\psi_{n+1} - z_n \psi_n}{z_n^{-1} - z_n} = \alpha_n \psi_{n+1} + \beta_n \psi_n$$

Derive self-energy

- Apply boundary points to difference equation

$$H\psi_1 = -s_1\psi_0 + d_1\psi_1 - s_2\psi_2 = E\psi_1$$

- From QTBM get relation:

$$\psi_0 = a_1 z_1^{-1} + b_1 z_1$$

$$b_1 = \psi_1 - a_1$$

- Substitute in difference equation:

$$E\psi_1 = -s_1 \left[a_1 z_1^{-1} + (\psi_1 - a_1) z_1 \right] + d_1 \psi_1 - s_2 \psi_2$$

$$E\psi_1 = -s_1 \psi_1 z_1 + s_1 (a_1 z_1 - a_1 z_1^{-1}) + d_1 \psi_1 - s_2 \psi_2$$

- Finally we get:

$$E\psi_1 = d_1 \psi_1 - s_2 \psi_2 \underbrace{- s_1 z_1 \psi_1}_{\text{self-energy}} + \underbrace{s_1 a_1 (z_1 - z_1^{-1})}_{\text{Source term}}$$

$$\Sigma = -s_1 z_1$$

$$S = s_1 a_1 (z_1 - z_1^{-1})$$

- Source term: excitation of channel by contact, depends on a_1 .
- Self-energy (not-hermitian): modification of H to incorporate BC.

General formulation in NEGF

- Schrodinger equation for isolated contact: $[EI_R - H_R]\{\Phi_R\} = \{0\}$
- Modified form:
 - » Extraction of electrons from contact $\rightarrow [i\eta]\{\Phi_R\}$
 - » Reinjection of electrons from external sources $\rightarrow \{S_R\}$
 - » Maintain constant electrochemical potential $\rightarrow [i\eta]\{\Phi_R\} = \{S_R\}$
- Impact: meaning of E changed...
 - » eigenenergy \rightarrow independent variable (energy of excitation from external source)
- Contact coupled to device:

$$\begin{pmatrix} EI_R - H_R + i\eta & -\tau^+ \\ -\tau & EI - H \end{pmatrix} \begin{Bmatrix} \Phi_R + \chi \\ \psi \end{Bmatrix} = \begin{Bmatrix} S_R \\ 0 \end{Bmatrix}$$
 - » Scattered waves $\{\chi\}$
 - » Coupling Hamiltonian $[\tau]$
- Substitute (f1) to eliminate S_R :

$$[EI_R - H_R + i\eta]\{\chi\} - [-\tau^+]\{\psi\} = \{0\}$$

$$[EI - H]\{\psi\} - [\tau]\{\chi\} = [\tau]\{\Phi_R\}$$
- Solve for $\{\chi\}$, get:

$$\{\chi\} = G_R \tau^+ \{\psi\}$$

$$G_R = [EI_R - H_R + i\eta]^{-1}$$

$$[\eta] = 0^+ [I_R]$$
 and

$$[EI - H - \Sigma]\{\psi\} = \{S\}$$

$$\Sigma = \tau G_R \tau^+$$

$$S = \tau \Phi_R$$

General formulation in NEGF

- G_R is of size R^2 , where R could be infinite
- $[\tau]$ is of size $(d \times R)$ and d is the size of device. ($d \ll R$)
- $[\tau]$ only couples r surface elements of contact to device
 - » $[\tau]$ could be $(d \times r)$ and $\rightarrow \Sigma = \tau g_R \tau^+ \quad S = \tau \phi_R$
 - » g_R is only a (r^2) subset of G_R , ϕ_R is $(r \times 1)$ subset of Φ_R

In 1D $r=1$

$$\tau = -s_1$$

$$\phi_R = -2ia_1 \sin(k\Delta)$$

$$g_R = -\frac{1}{s_1} z_1$$

$$S = s_1 a_1 (z_1 - z_1^{-1}) \quad \Sigma = -s_1 z_1$$

• Summary:

1. Channel with one contact:

$$\begin{pmatrix} EI_R - H_R + i\eta & -\tau^+ \\ -\tau & EI - H \end{pmatrix} \begin{Bmatrix} \Phi_R + \chi \\ \psi \end{Bmatrix} = \begin{Bmatrix} S_R \\ 0 \end{Bmatrix}$$

1. Equation only for the channel:

$$[EI - H - \Sigma] \{\psi\} = \{S\} \quad \Sigma = \tau G_R \tau^+ = \Sigma^R$$

2. Solution: $\{\psi\} = [G] \{S\}$ with

$$[G] = [EI - H - \Sigma]^{-1}$$

• NEGF equations:

» Channel with two contacts:

$$[EI - H - \Sigma_1 - \Sigma_2] \{\psi\} = \{S\}$$

» Channel Green's function:

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

» Electron density:

$$[G^n] = G \Sigma^{in} G^+ = [G^<]$$

» In scattering:

$$\Sigma^{in} = \{S\} \{S\}^+ = \Sigma^<$$