NEGF in a Quasi-1D formulation

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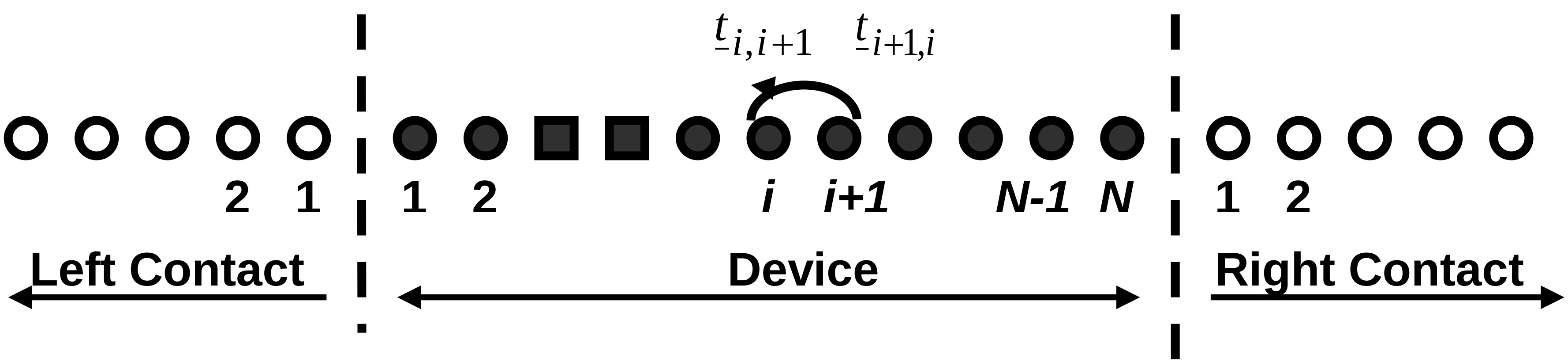
NEGF in a Quasi-1D formulation

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

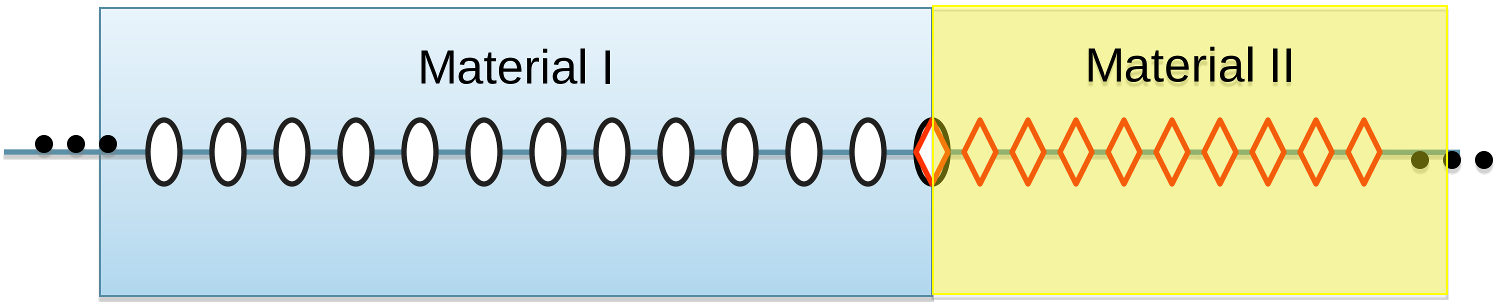
$$\frac{\partial^2\psi}{\partial x^2} \approx \frac{\psi(x-\Delta) - 2\psi(x) + \psi(x+\Delta)}{\Delta^2}$$

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

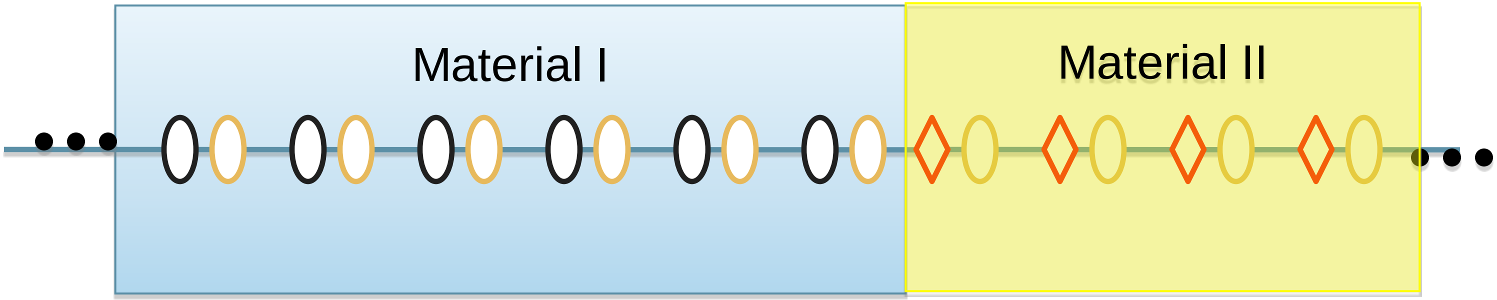
- If m*(x) is allowed to vary… which is real in heterostructure
  - » Variation will be included in values of s_j, d_j (continued…)

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)

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

$$s_j = \frac{\hbar^2}{2\Delta^2 m^*_{j+\frac{1}{2}}}$$

1

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

$$s_j = \frac{\hbar^2}{4\Delta^2}\left(\frac{1}{m^*_{j-1}} + \frac{1}{m^*_j}\right)$$

2

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

$$s_j = \frac{\hbar^2}{\Delta^2}\frac{1}{m^*_{j-1} + m^*_j}$$

3

Hamiltonian for a close system

$$
\begin{bmatrix}
d_1 - E & -s_2 & & & & & & & & \\
-s_2 & d_2 - E & -s_3 & & & & & & & \\
 & -s_3 & d_3 - E & -s_4 & & & & & & \\
 & & \cdot & \cdot & \cdot & & & & & \\
 & & & \cdot & \cdot & \cdot & & & & \\
 & & & & \cdot & \cdot & \cdot & & & \\
 & & & & & \cdot & \cdot & \cdot & & \\
 & & & & & & \cdot & \cdot & \cdot & \\
 & & & & & & & -s_{n-1} & d_{n-1} - E & -s_n \\
 & & & & & & & & -s_n & d_n
\end{bmatrix}
\begin{bmatrix}
\psi_1 \\ \psi_2 \\ \psi_3 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \psi_{n-1} \\ \psi_n
\end{bmatrix}
=
\begin{bmatrix}
0 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ 0
\end{bmatrix}
$$

- Diagonalize this tridiagonal H to get eigenstates of a closed system.
- Open system not enough…(continued…)

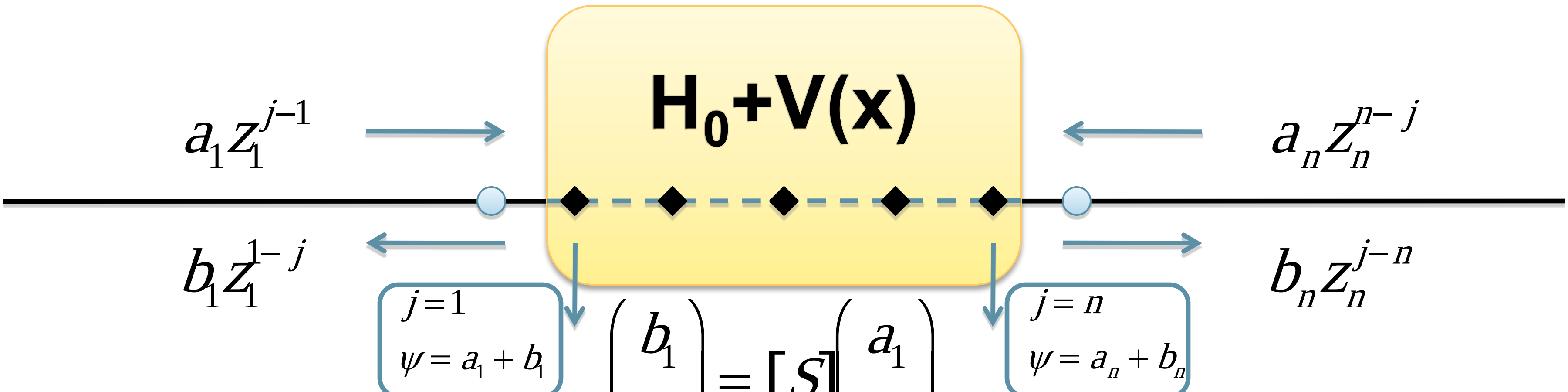
Quantum Transmitting Boundary Method (QTBM) in discrete case

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

$$j \le 1 \ldots\ldots \psi_j = a_1 z_1^{j-1} + b_1 z_1^{1-j}$$

$$j \ge n \ldots\ldots \psi_j = a_n z_n^{n-j} + b_n z_n^{j-n}$$

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



$$\begin{pmatrix} b_1 \\ b_n \end{pmatrix} = [S] \begin{pmatrix} a_1 \\ a_n \end{pmatrix}$$

- Scattering Matrix: [S]

Quantum Transmitting Boundary Method (QTBM) in discrete case

- To get z, substitute to difference equation:
  - » solve for z, z_n:

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

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

- 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 ➔

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

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

Hamiltonian with QTBM

$$\begin{bmatrix} \alpha_1 & \beta_1 & & & & & & & \\ -s_1 & d_1 - E & -s_2 & & & & & & \\ & -s_2 & d_2 - E & -s_3 & & & & & \\ & & \cdot & \cdot & \cdot & & & & \\ & & & \cdot & \cdot & \cdot & & & \\ & & & & \cdot & \cdot & \cdot & & \\ & & & & & \cdot & \cdot & \cdot & \\ & & & & & & -s_n & d_n - E & -s_{n+1} \\ & & & & & & & \beta_n & \alpha_n \end{bmatrix} \begin{bmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \psi_n \\ \psi_{n+1} \end{bmatrix} = \begin{bmatrix} a_1 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ a_n \end{bmatrix}$$

- Add QTBM equation to matrix representation Sch-equ Hamiltonian
  - » to find left scattering state → a_1=1 and a_n=0 (for right conversely)

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:

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

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

- Finally we get:

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

$$\Sigma = -s_1 z_1$$

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

- 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:

  $[EI_R - H_R + i\eta]\{\Phi_R\} = \{S_R\}$ - - - (f1)

  » Extraction of electrons from contact → $[i\eta]\{\Phi_R\}$

  » Reinjection of electrons from external sources → $\{S_R\}$

  » Maintain constant electrochemical potential → $[i\eta]\{\Phi_R\} = \{S_R\}$
- Impact: meaning of E changed…

  » eigenenergy ➔ 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 { χ }

  » Coupling Hamiltonian [τ]
- 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 { χ }, 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

In 1D r=1

$\tau = -s_1$

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

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

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

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