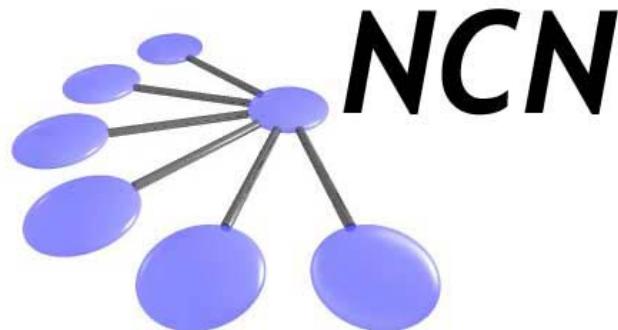


# *Network for Computational Nanotechnology (NCN)*

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

# Recursive Green Function Algorithm

Gerhard Klimeck



- Dynamics - States of the System - NEGF:  $G^R$

» Need to solve a form of the Schrödinger Wave Equation.

$$(E - H - \Sigma_{\text{bound}}^R - \Sigma_{\text{scatt}}^R) G^R = 1 \quad G^R \quad \text{impulse response}$$

$$\Sigma_{\text{bound}}^R = \Gamma^{\text{left}} + \Gamma^{\text{right}} \quad \Sigma_{\text{bound}}^R \quad \text{out-scattering to contacts}$$

$$\Sigma_{\text{scatt}}^R = D_x G^R \quad \Sigma_{\text{scatt}}^R \quad \text{out-scattering to other channels}$$

- Kinetics - Occupation of states - transfer of carriers - NEGF:  $G^<$

» Need to account for many electrons, injection from contacts, scattering

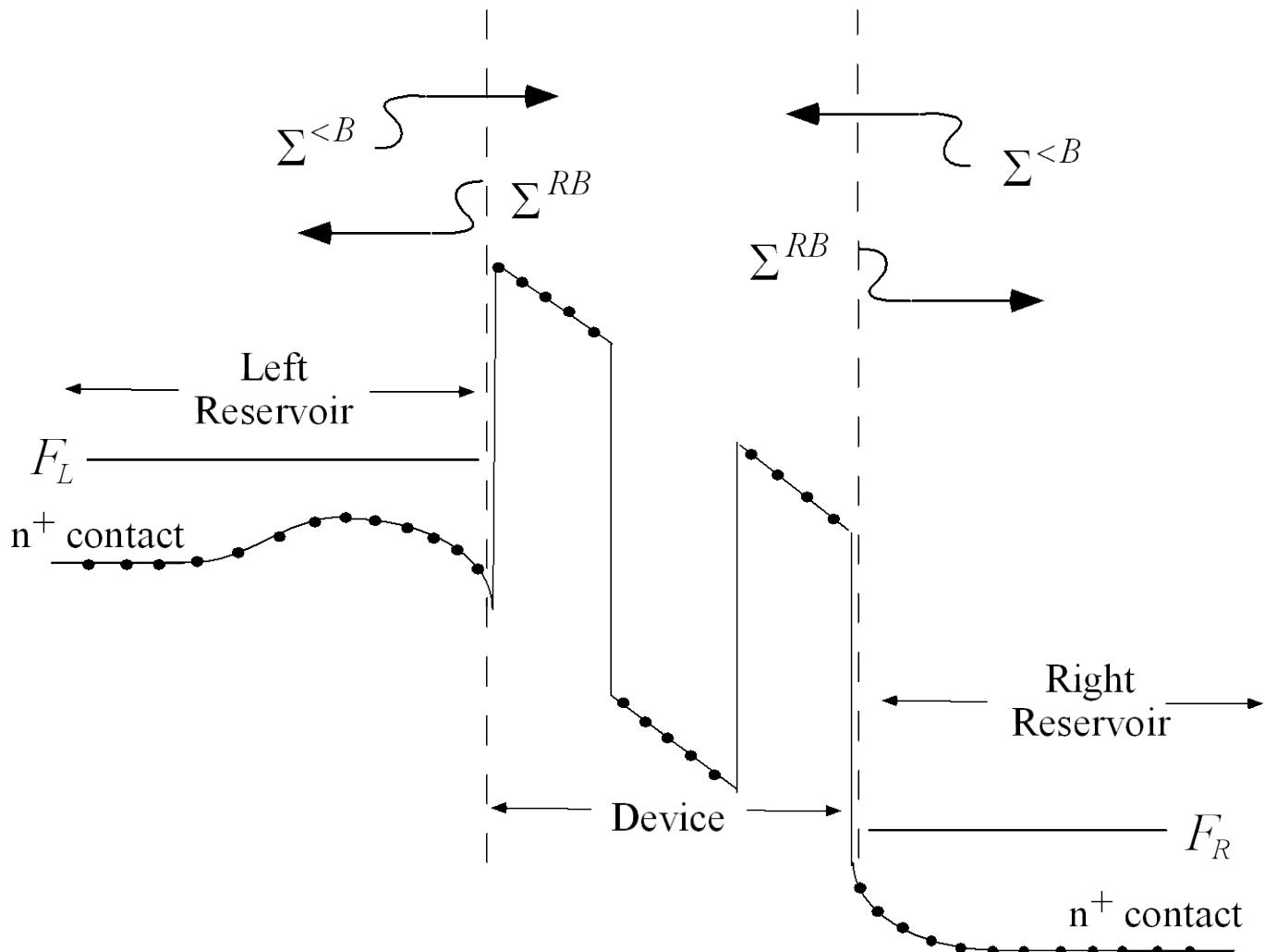
$$G^< = G^R (\Sigma_{\text{bound}}^< + \Sigma_{\text{scatt}}^<) G^{R+}$$

$$\Sigma_{\text{bound}}^< = \Gamma^{\text{left}} f^{\text{left}} + \Gamma^{\text{right}} f^{\text{right}} \quad \Sigma_{\text{bound}}^< \quad \text{in-scattering from boundaries}$$

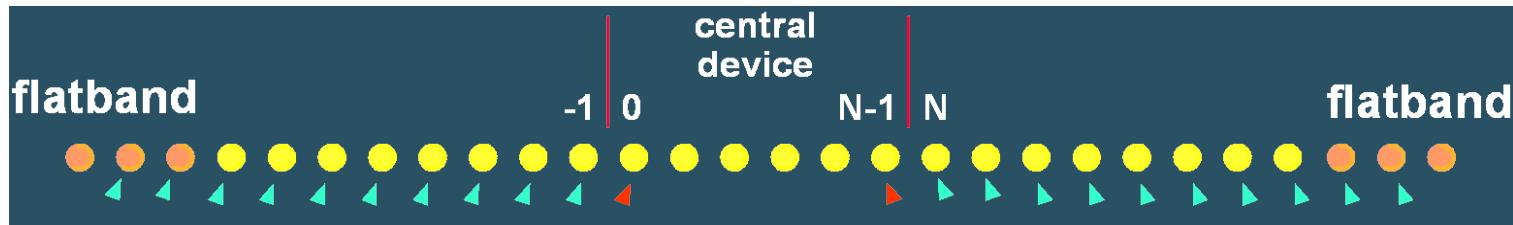
$$\Sigma_{\text{scatt}}^< = D_x G^< \quad \Sigma_{\text{scatt}}^< \quad \text{in-scattering from other channels}$$

# Three Critical Simulation Domains:

left reservoir, central device, right reservoir



# Dyson Equation Treatment of the Leads



$$\Sigma_{0,0}^{RB} = g_{-1,-1}^R |t_{-1,0}|^2$$

$$\Sigma_{N-1,N-1}^{RB} = g_{N,N}^R |t_{N,N-1}|^2$$

$$\Sigma_{0,0}^{<B} = -2 \text{ IM } \left\{ \Sigma_{0,0}^{RB} \right\} f_L$$

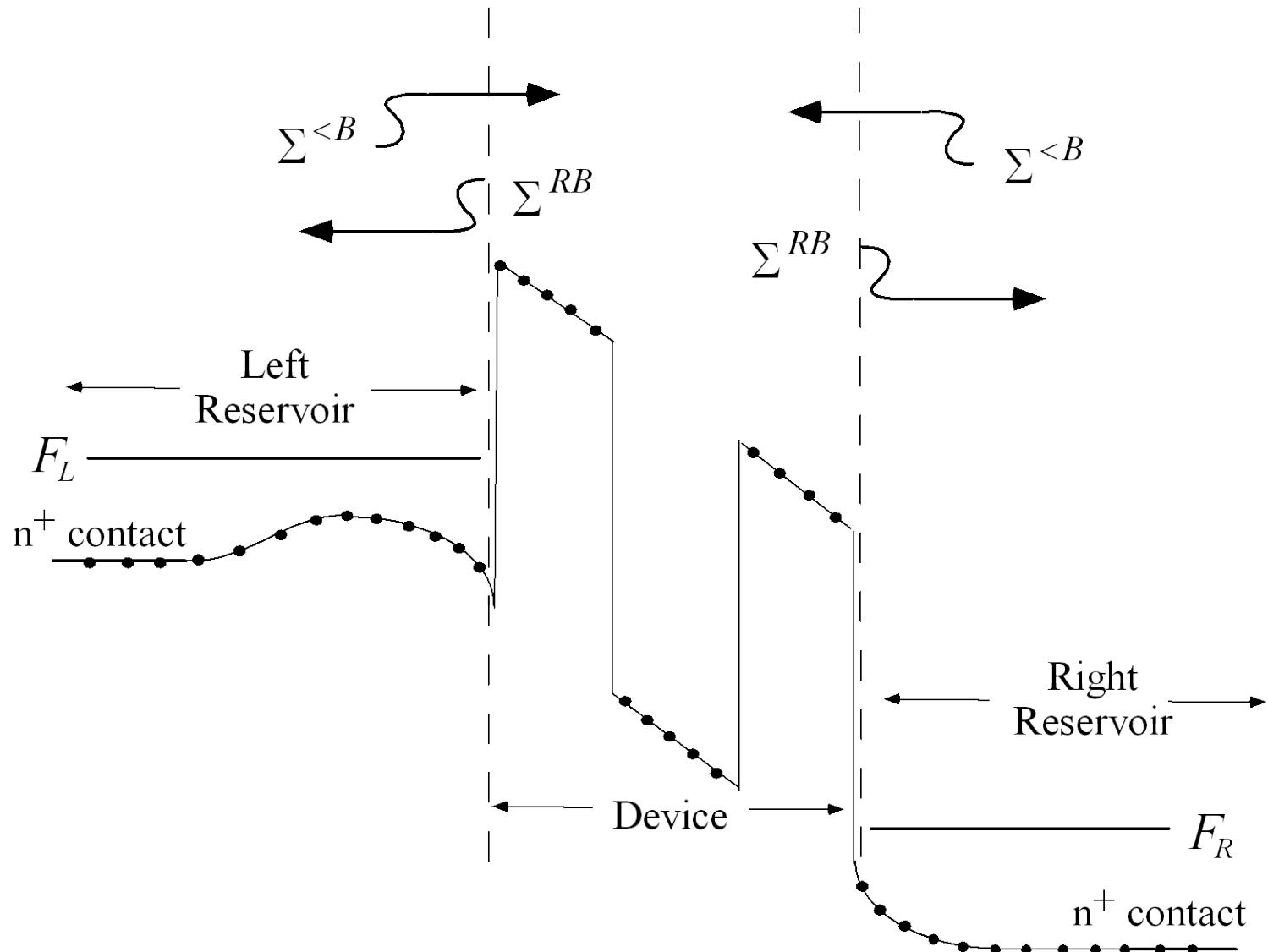
$$\Sigma_{N-1,N-1}^{<B} = -2 \text{ IM } \left\{ \Sigma_{N-1,N-1}^{RB} \right\} f_R$$

$$\left[ G^R \right]^{-1} = \begin{bmatrix} E - \varepsilon_0 - \Sigma_{0,0}^R & t_{0,1} & & \\ t_{1,0} & E - \varepsilon_1 & \ddots & \\ & \ddots & \ddots & \\ & & & E - \varepsilon_{N-1} - \Sigma_{N-1,N-1}^R \end{bmatrix}^{-1}$$

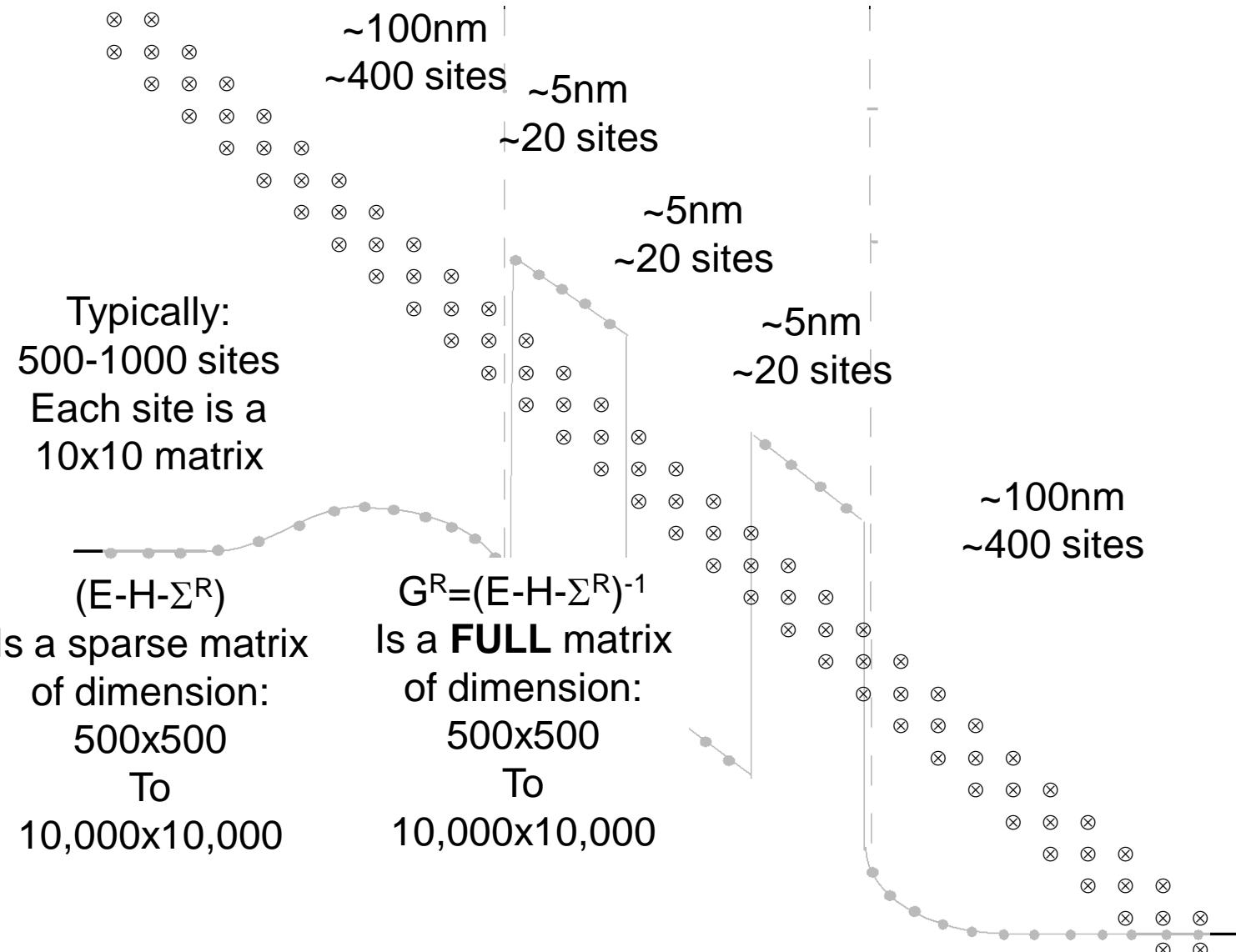
$$(E - H_0 - \Sigma^{RB}) G^R = 1$$

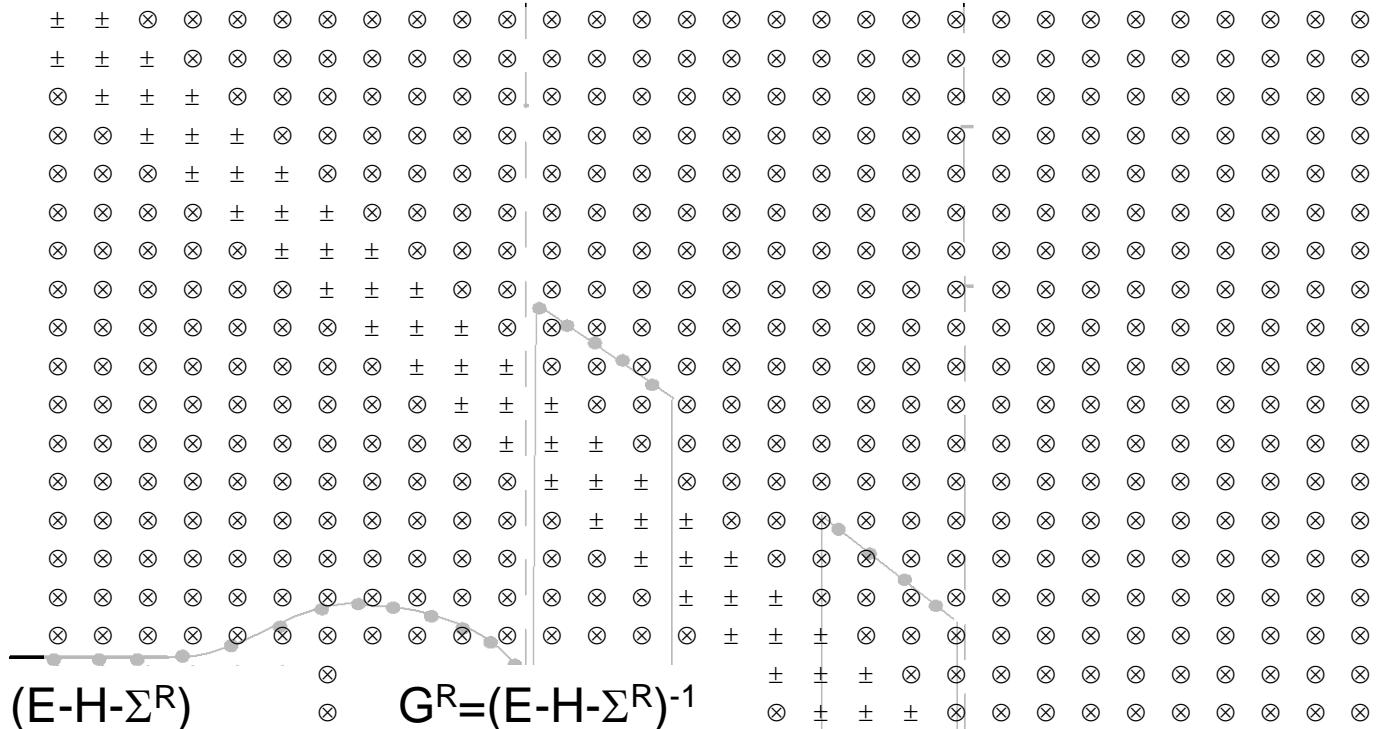
$$(E - H_0 - \Sigma^{RB}) G^< = \Sigma^{<B} G^A$$

$$\begin{array}{ccccccc}
 E - \varepsilon_0 & & t_{0,1} & & & & \\
 & t_{1,0} & E - \varepsilon_1 & t_{1,2} & & & \\
 & & t_{2,1} & E - \varepsilon_2 & t_{2,3} & & \\
 & & t_{3,2} & E - \varepsilon_3 & t_{3,4} & & \\
 & & t_{4,3} & E - \varepsilon_4 & \cdot & & \\
 & & & & \cdot & \cdot & \cdot \\
 & & & & \cdot & \cdot & \cdot \\
 & & & & \cdot & E - \varepsilon_{N-3} & t_{N-3, N-2} \\
 & & & & t_{N-2, N-3} & E - \varepsilon_{N-2} & t_{N-2, N-1} \\
 & & & & t_{N-1, N-2} & E - \varepsilon_{N-1} &
 \end{array}$$



# Each Atomic Layer is Represented





$\otimes$   $(E - H - \Sigma^R)$   
 Is a sparse matrix  
 of dimension:  
 $500 \times 500$   
 To  
 $10,000 \times 10,000$

$\otimes$  Storage:  
 $10,000 \times 3 \times 16B =$   
**0.5MB**

$\otimes$   $G^R = (E - H - \Sigma^R)^{-1}$   
 Is a **FULL** matrix  
 of dimension:  
 $500 \times 500$   
 To  
 $10,000 \times 10,000$   
 $\otimes$  Storage:  
 $10,000 \times 10,000 \times 16B =$   
**1600MB**

# Full Matrix Inversion is Expensive

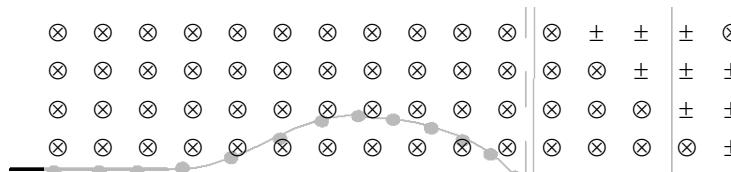
$\pm \pm \otimes \otimes \otimes \otimes \otimes | \otimes \otimes$

$$G^R = (E - H - \Sigma^R)^{-1}$$

- standard operation count:  $N^3 = 10^{12}$  ops. 3.2 years
- Tri-diag LU:  $N^2 = 10^8$  ops. 2.7 hr

May not need all matrix elements:

- Recursive Green Fct.:  $N^1 = 10^4$  ops. 1 sec.



$$(E - H - \Sigma^R)$$

Is a sparse matrix  
of dimension:

$$500 \times 500$$

To  
 $10,000 \times 10,000$

Storage:

$$10,000 \times 3 \times 16B =$$

$$0.5MB$$

$$G^R = (E - H - \Sigma^R)^{-1}$$

Is a **FULL** matrix  
of dimension:

$$500 \times 500$$

To  
 $10,000 \times 10,000$

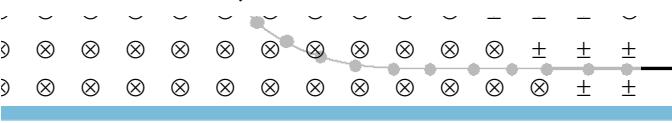
Storage:

$$10,000 \times 10,000 \times 16B =$$

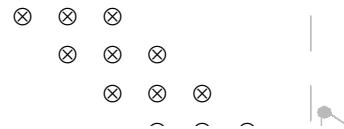
$$1600MB$$

Once is not enough:  
 -need 100-1000 energies  
 -for 5-7 iterations  
 -For 10-100 bias points

=> Need  $G^R$  about  
165,000 times!

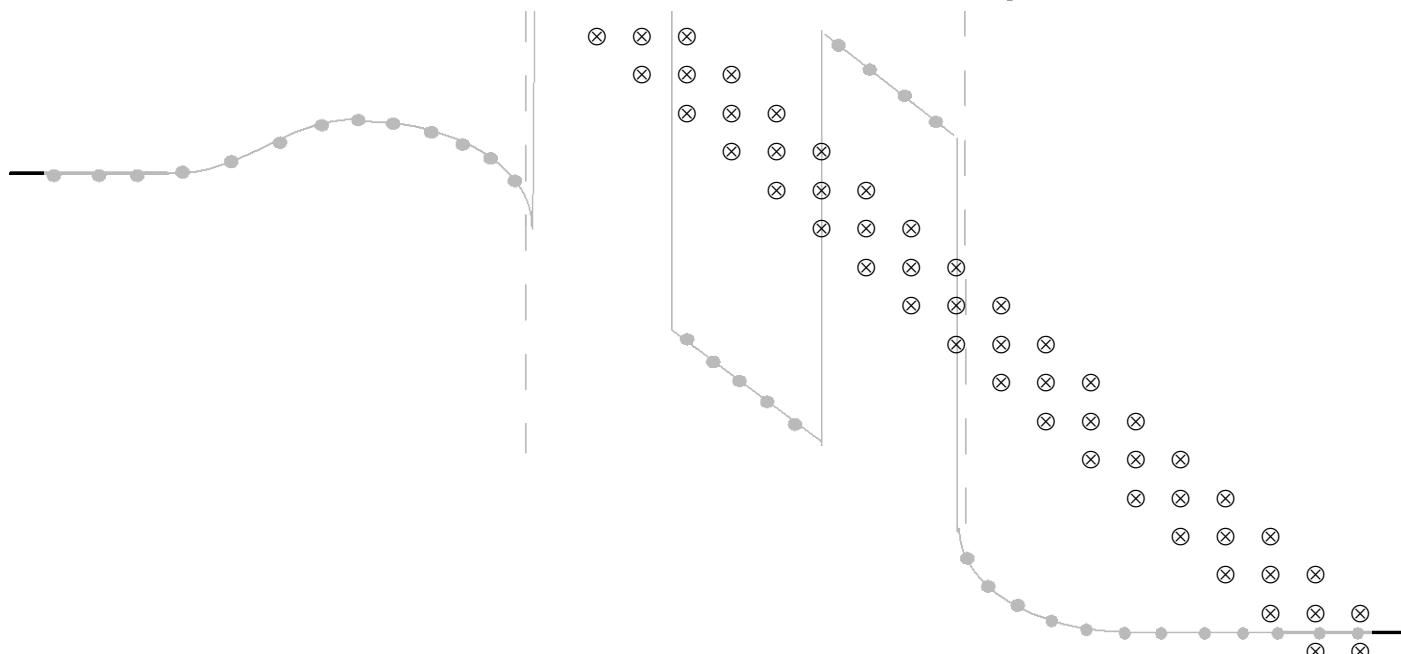


$$G^R = (E - H - \Sigma^R)^{-1}$$



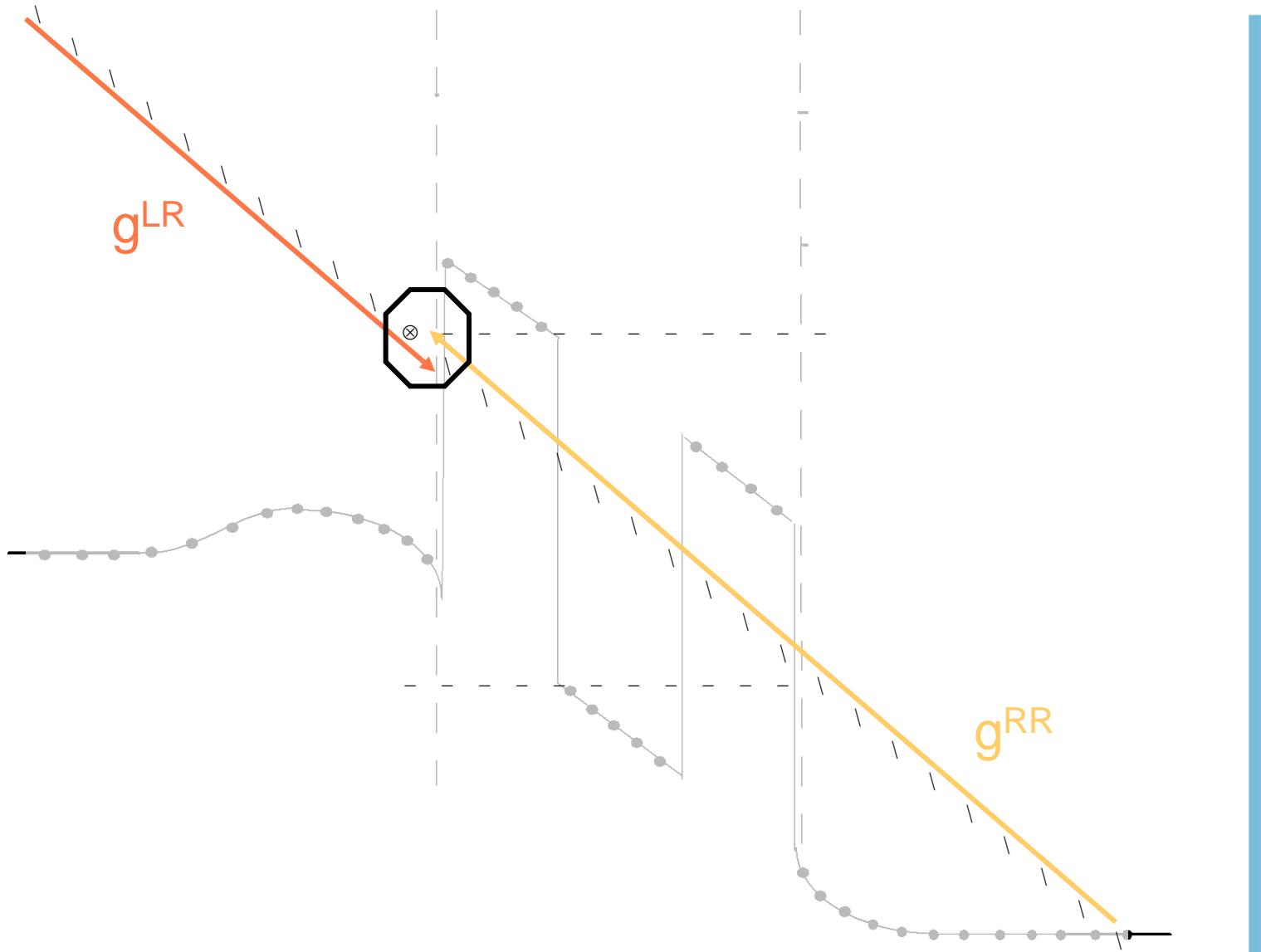
May not need all matrix elements:

-Recursive Green Fct.:  $N^1=10^4$  ops. 1 sec.



- No incoherent scattering:  $(E-H-\Sigma^R_{\text{bound}}) G^R = 1$
- » No charge effects:
  - ✓ Boundary conditions.  $g^R_{\text{left},\text{left}} g^R_{\text{right},\text{right}}$
  - ✓ Current on ONE site.  $J \sim G^R_{i,i}$

Details in: Lake, Klimeck, Bowen and Jovanovic, J. of Appl. Phys. 81, 7845 (1997).



- No incoherent scattering:  $(E-H-\Sigma^R_{\text{bound}}) G^R = 1$

## » No charge effects:

- ✓ Boundary conditions.
- ✓ Current on ONE site.

$$g^R_{\text{left},\text{left}} g^R_{\text{right},\text{right}} \\ J \sim G^R_{i,i}$$

## » With charge effects:

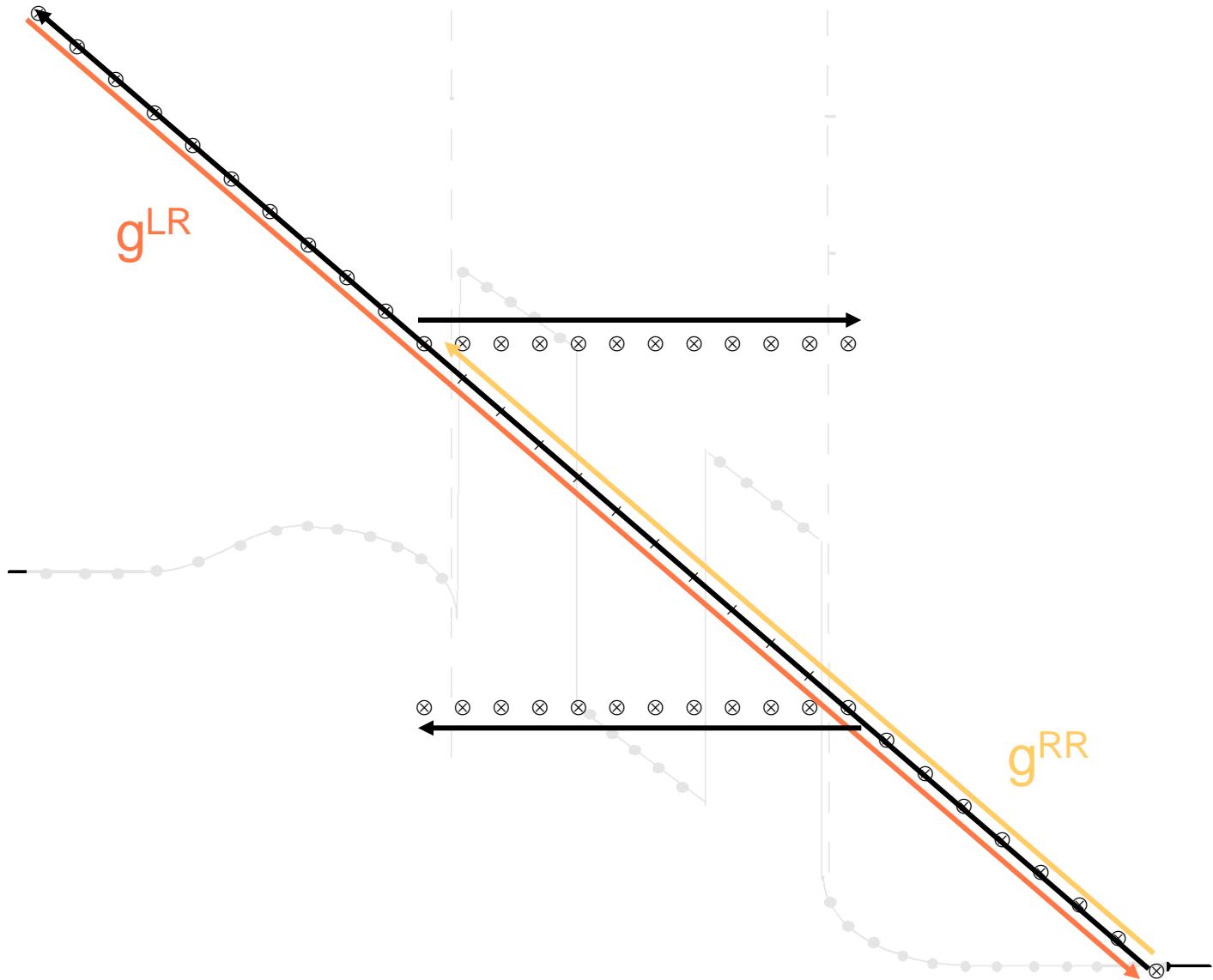
- ✓ Boundary conditions.
- ✓ Current on one site.
- ✓ Charge throughout the
  - non-equilibrium device:
  - device reservoirs:

$$g^R_{\text{left},\text{left}} g^R_{\text{right},\text{right}} \\ J \sim G^R_{i,i} \\ N \sim \sum_j (G^R_{I,j}) + \sum_j (G^R_{K,j}) \\ N \sim G^R_{i,i}$$

Details in: Lake, Klimeck, Bowen and Jovanovic, J. of Appl. Phys. 81, 7845 (1997).

# Current and Charge?

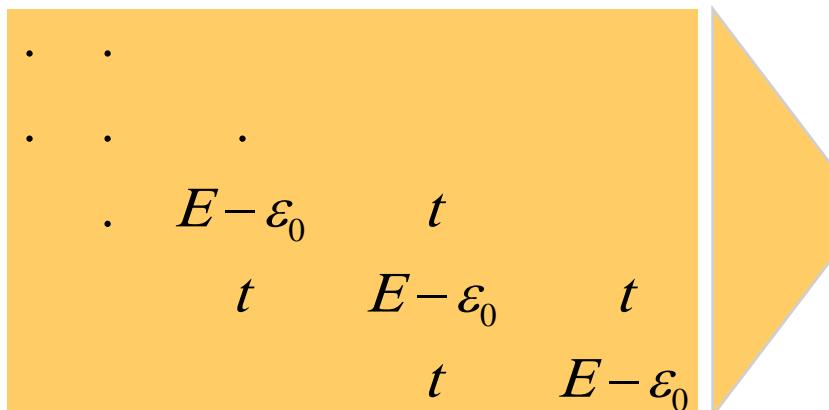
=> 2 diagonals in reservoirs, 2 off-diagonals in center



$$\begin{array}{ccccccc}
 E - \varepsilon_0 & & t_{0,1} & & & & \\
 & t_{1,0} & E - \varepsilon_1 & t_{1,2} & & & \\
 & & t_{2,1} & E - \varepsilon_2 & t_{2,3} & & \\
 & & t_{3,2} & E - \varepsilon_3 & t_{3,4} & & \\
 & & t_{4,3} & E - \varepsilon_4 & . & & \\
 & & & & \ddots & & \\
 & & & & & \ddots & \\
 & & & & & & \ddots \\
 & & & & & E - \varepsilon_{N-3} & t_{N-3,N-2} \\
 & & & & & t_{N-2,N-3} & E - \varepsilon_{N-2} & t_{N-2,N-1} \\
 & & & & & t_{N-1,N-2} & E - \varepsilon_{N-1} &
 \end{array}$$

$E - \varepsilon_0 - \Sigma^R_{0,0}$	$t_{0,1}$							
$t_{1,0}$	$E - \varepsilon_1$	$t_{1,2}$						
	$t_{2,1}$	$E - \varepsilon_2$	$t_{2,3}$					
	$t_{3,2}$	$E - \varepsilon_3$	$t_{3,4}$					
	$t_{4,3}$	$E - \varepsilon_4$	.					
	.	.	.	.	.			
	.	.	.	.	.	$E - \varepsilon_{N-3}$	$t_{N-3,N-2}$	
						$t_{N-2,N-3}$	$E - \varepsilon_{N-2}$	$t_{N-2,N-1}$
						$t_{N-1,N-2}$	$E - \varepsilon_{N-1} - \Sigma^R_{N-1,N-1}$	

$\Sigma^R_{0,0}$  computed semi-analytically from infinitely periodic left open



$$E - \varepsilon_0 - \Sigma^R_{0,0}$$

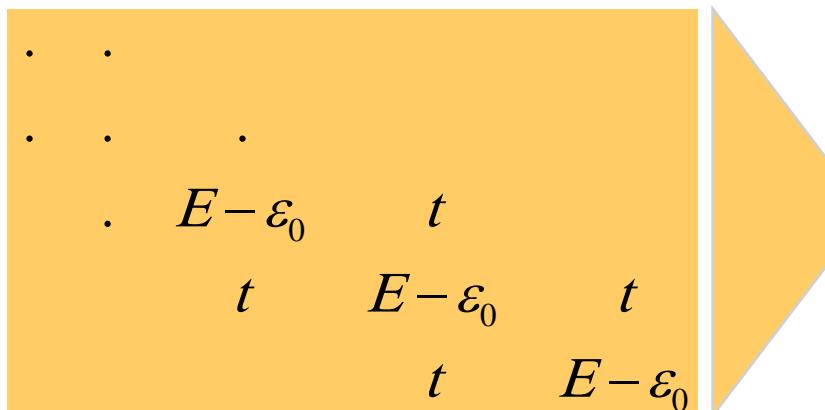
$$(E - \varepsilon_0 - \Sigma^R_{0,0}) g^R_{0,0} = 1$$

$$\begin{matrix}
 E - \varepsilon_0 - \Sigma_{0,0}^R & & t_{0,1} \\
 & t_{1,0} & E - \varepsilon_1 & t_{1,2} \\
 & t_{2,1} & E - \varepsilon_2 & t_{2,3} \\
 & t_{3,2} & E - \varepsilon_3 & t_{3,4} \\
 & t_{4,3} & E - \varepsilon_4 & . \\
 & \cdot & \cdot & \cdot \\
 & \cdot & \cdot & \cdot \\
 & \cdot & \cdot & \cdot \\
 & E - \varepsilon_{N-3} & t_{N-3,N-2} \\
 t_{N-2,N-3} & E - \varepsilon_{N-2} & & t_{N-2,N-1} \\
 t_{N-1,N-2} & E - \varepsilon_{N-1} - \Sigma_{N-1,N-1}^R & &
 \end{matrix}$$

$$\begin{array}{ccccccc}
 E - \varepsilon_0 & & t_{0,1} & & & & \\
 & t_{1,0} & E - \varepsilon_1 & t_{1,2} & & & \\
 & & t_{2,1} & E - \varepsilon_2 & t_{2,3} & & \\
 & & t_{3,2} & E - \varepsilon_3 & t_{3,4} & & \\
 & & t_{4,3} & E - \varepsilon_4 & . & & \\
 & & & & \ddots & & \\
 & & & & & \ddots & \\
 & & & & & & \ddots \\
 & & & & & E - \varepsilon_{N-3} & t_{N-3,N-2} \\
 & & & & & t_{N-2,N-3} & E - \varepsilon_{N-2} & t_{N-2,N-1} \\
 & & & & & t_{N-1,N-2} & E - \varepsilon_{N-1} & 
 \end{array}$$

$E - \varepsilon_0 - \Sigma_{0,0}^R$	$t_{0,1}$													
$t_{1,0}$	$E - \varepsilon_1$	$t_{1,2}$												
	$t_{2,1}$	$E - \varepsilon_2$	$t_{2,3}$											
		$t_{3,2}$	$E - \varepsilon_3$	$t_{3,4}$										
		$t_{4,3}$	$E - \varepsilon_4$	.										
			.	.	.	.	.	.	.					
			.	.	.	.	.	.	.	$E - \varepsilon_{N-3}$	$t_{N-3,N-2}$			
			.	.	.	.	.	.	.	$t_{N-2,N-3}$	$E - \varepsilon_{N-2}$	$t_{N-2,N-1}$		
			.	.	.	.	.	.	.	$t_{N-1,N-2}$	$E - \varepsilon_{N-1} - \Sigma_{N-1,N-1}^R$			

$\Sigma_{0,0}^R$  computed semi-analytically from infinitely periodic left open



$$E - \varepsilon_0 - \Sigma_{0,0}^R \quad (E - \varepsilon_0 - \Sigma_{0,0}^R) g_{0,0}^R = 1$$

$$\left( \begin{array}{ccccccccc}
 D_0 & t_{0,1} & & & & & & & \\
 t_{1,0} & D_1 & t_{i+1,i+2} & & & & & & \\
 & t_{i+2,i+1} & D_2 & t_{i+2,i+3} & & & & & \\
 & & t_{i+3,i+2} & D_3 & t_{i+3,i+4} & & & & \\
 & & t_{i+4,i+3} & D_4 & & \cdot & & & \\
 & & & \cdot & \cdot & \cdot & & & \\
 & & & & \cdot & \cdot & \cdot & & \\
 & & & & & \cdot & D_{N-3} & t_{N-3,N-2} & \\
 & & & & & t_{N-2,N-3} & D_{N-2} & t_{N-1,N-2} & \\
 & & & & & t_{N-2,N-1} & D_{N-1} & & 
 \end{array} \right) G^R = 1$$

$$D_0 g_{0,0}^{LR} = 1$$

left connected  $g^R$

$$D_{N-1} g_{N-1,N-1}^{RR} = 1$$

right connected  $g^R$

Need some elements of fully connected  $G^R$

$$g_{0,0}^{LR} = (D_0)^{-1}$$

$$g_{1,1}^{LR} = (D_1 - t_{1,0} g_{0,0}^{LR} t_{0,1})^{-1}$$

$$D_0$$

$$g_{0,0}^{LR} = (D_0)^{-1}$$

$$D_0 \quad t_{0,1}$$

$$g_{1,1}^{LR} = (D_1 - t_{1,0} g_{0,0}^{LR} t_{0,1})^{-1}$$

$$t_{1,0} \quad D_1 \quad t_{1,2}$$

$$g_{2,2}^{LR} = (D_2 - t_{2,1} g_{1,1}^{LR} t_{1,2})^{-1}$$

$$t_{2,1} \quad D_2$$

$$g_{0,0}^{LR} = (D_0)^{-1}$$

$$D_0 \quad t_{0,1}$$

$$g_{1,1}^{LR} = (D_1 - t_{1,0} g_{0,0}^{LR} t_{0,1})^{-1}$$

$$t_{1,0} \quad D_1 \quad t_{1,2}$$

$$g_{2,2}^{LR} = (D_2 - t_{2,1} g_{1,1}^{LR} t_{1,2})^{-1}$$

$$t_{2,1} \quad D_2 \quad t_{2,3}$$

$$g_{3,3}^{LR} = (D_3 - t_{3,2} g_{2,2}^{LR} t_{2,3})^{-1}$$

$$t_{3,2} \quad D_3$$

$$\begin{array}{ll}
 g_{0,0}^{LR} = (D_0)^{-1} & D_0 \quad t_{0,1} \\
 g_{1,1}^{LR} = (D_1 - t_{1,0} g_{0,0}^{LR} t_{0,1})^{-1} & t_{1,0} \quad D_1 \quad t_{1,2} \\
 g_{2,2}^{LR} = (D_2 - t_{2,1} g_{1,1}^{LR} t_{1,2})^{-1} & t_{2,1} \quad D_2 \quad t_{2,3} \\
 g_{3,3}^{LR} = (D_3 - t_{3,2} g_{2,2}^{LR} t_{2,3})^{-1} & t_{3,2} \quad D_3 \quad t_{3,4} \\
 & t_{4,3} \quad D_4 \quad \cdot \\
 & \cdot \quad \cdot \quad \cdot \\
 & \cdot \quad \cdot \quad \cdot
 \end{array}$$

$$g_{i,i}^{LR} = (D_i - t_{i,i-1} g_{i-1,i-1}^{LR} t_{i-1,i})^{-1}$$

$$g_{0,0}^{LR} = (D_0)^{-1}$$

$$D_0 \quad t_{0,1}$$

$$g_{1,1}^{LR} = (D_1 - t_{1,0} g_{0,0}^{LR} t_{0,1})^{-1}$$

$$t_{1,0} \quad D_1 \quad t_{1,2}$$

$$g_{2,2}^{LR} = (D_2 - t_{2,1} g_{1,1}^{LR} t_{1,2})^{-1}$$

$$t_{2,1} \quad D_2 \quad t_{2,3}$$

$$g_{3,3}^{LR} = (D_3 - t_{3,2} g_{2,2}^{LR} t_{2,3})^{-1}$$

$$t_{3,2} \quad D_3 \quad t_{3,4}$$

$$t_{4,3} \quad D_4 \quad \cdot$$

$$\cdot \quad \cdot \quad \cdot$$

$$g_{i,i}^{LR} = (D_i - t_{i,i-1} g_{i-1,i-1}^{LR} t_{i-1,i})^{-1}$$

$$\begin{matrix} & & & & \cdot & \cdot & \cdot \\ & & & & \cdot & \cdot & \cdot \\ & & & & \cdot & D_{N-3} & t_{N-3,N-2} \\ & & & & \cdot & t_{N-2,N-3} & D_{N-2} & t_{N-1,N-2} \\ & & & & & t_{N-2,N-1} & D_{N-1} \end{matrix}$$

$$g_{N-1,N-1}^{LR} = (D_{N-1} - t_{N-1,N-2} g_{N-2,N-2}^{LR} t_{N-2,N-1})^{-1}$$

$$D_{N-1} = (g_{N-1,N-1}^{RR})^{-1}$$

The last block is special:  
 It is the right-connected exact solution!  
 Left-connected and right-connected matrix  
 meet at the last site!

$$\begin{aligned} g_{0,0}^{LR} &= (D_0)^{-1} \\ g_{1,1}^{LR} &= (D_1 - t_{1,0} g_{0,0}^{LR} t_{0,1})^{-1} \\ g_{2,2}^{LR} &= (D_2 - t_{2,1} g_{1,1}^{LR} t_{1,2})^{-1} \\ g_{3,3}^{LR} &= (D_3 - t_{3,2} g_{2,2}^{LR} t_{2,3})^{-1} \end{aligned}$$

$$\begin{array}{ccccccccc} D_0 & t_{0,1} & & & & & & & \\ t_{1,0} & D_1 & t_{1,2} & & & & & & \\ & t_{2,1} & D_2 & t_{2,3} & & & & & \\ & & t_{3,2} & D_3 & t_{3,4} & & & & \\ & & & t_{4,3} & D_4 & \cdot & & & \\ & & & & & \cdot & \cdot & \cdot & \\ & & & & & & \cdot & \cdot & \cdot \\ & & & & & & & D_{N-3} & t_{N-3,N-2} \\ & & & & & & & t_{N-2,N-3} & D_{N-2} & t_{N-1,N-2} \\ & & & & & & & & t_{N-2,N-1} & D_{N-1} \end{array}$$

$$g_{N-1,N-1}^{LR} = (D_{N-1} - t_{N-1,N-2} g_{N-2,N-2}^{LR} t_{N-2,N-1})^{-1} = G_{N-1,N-1}^R \quad \text{One block of } G^R: G_{N-1,N-1}^R$$

$$D_{N-1} = (g_{N-1,N-1}^{RR})^{-1}$$

The last block is special:  
It is the right-connected exact solution!  
Left-connected and right-connected matrix  
meet at the last site!

$$\begin{array}{ccccccc}
 g_{0,0}^{LR} & & t_{0,1} & & & & \\
 t_{1,0} & g_{1,1}^{LR} & t_{1,2} & & & & \\
 & t_{2,1} & g_{2,2}^{LR} & t_{2,3} & & & \\
 & & t_{3,2} & g_{3,3}^{LR} & t_{3,4} & & \\
 & & & t_{4,3} & g_{4,4}^{LR} & \cdot & \\
 & & & & \cdot & \cdot & \\
 & & & & & g_{N-3,N-3}^{LR} & t_{N-3,N-2} \\
 & & & & & t_{N-2,N-3} & g_{N-2,N-2}^{LR} & t_{N-1,N-2} \\
 & & & & & t_{N-2,N-1} & G_{N-1,N-1}^R
 \end{array}$$

$$g_{i,i}^{LR} = \left( D_i - t_{i,i-1} g_{i-1,i-1}^{LR} t_{i-1,i} \right)^{-1}$$

$$g_{N-1,N-1}^{LR} = \left( D_{N-1} - t_{N-1,N-2} g_{N-2,N-2}^{LR} t_{N-2,N-1} \right)^{-1} = G_{N-1,N-1}^R$$

One block of  $G^R$ :  $G_{N-1,N-1}^R$

$$\begin{array}{c}
 g^{LR}_{N-2,N-2} & t_{N-1,N-2} \\
 t_{N-2,N-1} & G^R_{N-1,N-1}
 \end{array}$$

## Backward Recursion:

$$G^R_{N-2,N-2} = g^{LR}_{N-2,N-2} \left( 1 + t_{N-2,N-1} G^R_{N-1,N-1} t_{N-1,N-2} g^{LR}_{N-2,N-2} \right) G^R_{N-2,N-2} \text{ from } G^R_{N-1,N-1} \text{ and } g^{LR}_{N-2,N-2}$$

$$g_{N-3,N-3}^{LR}$$

$$t_{N-3,N-2}$$

$$t_{N-2,N-3}$$

$$G_{N-2,N-2}^R$$

$$t_{N-1,N-2}$$

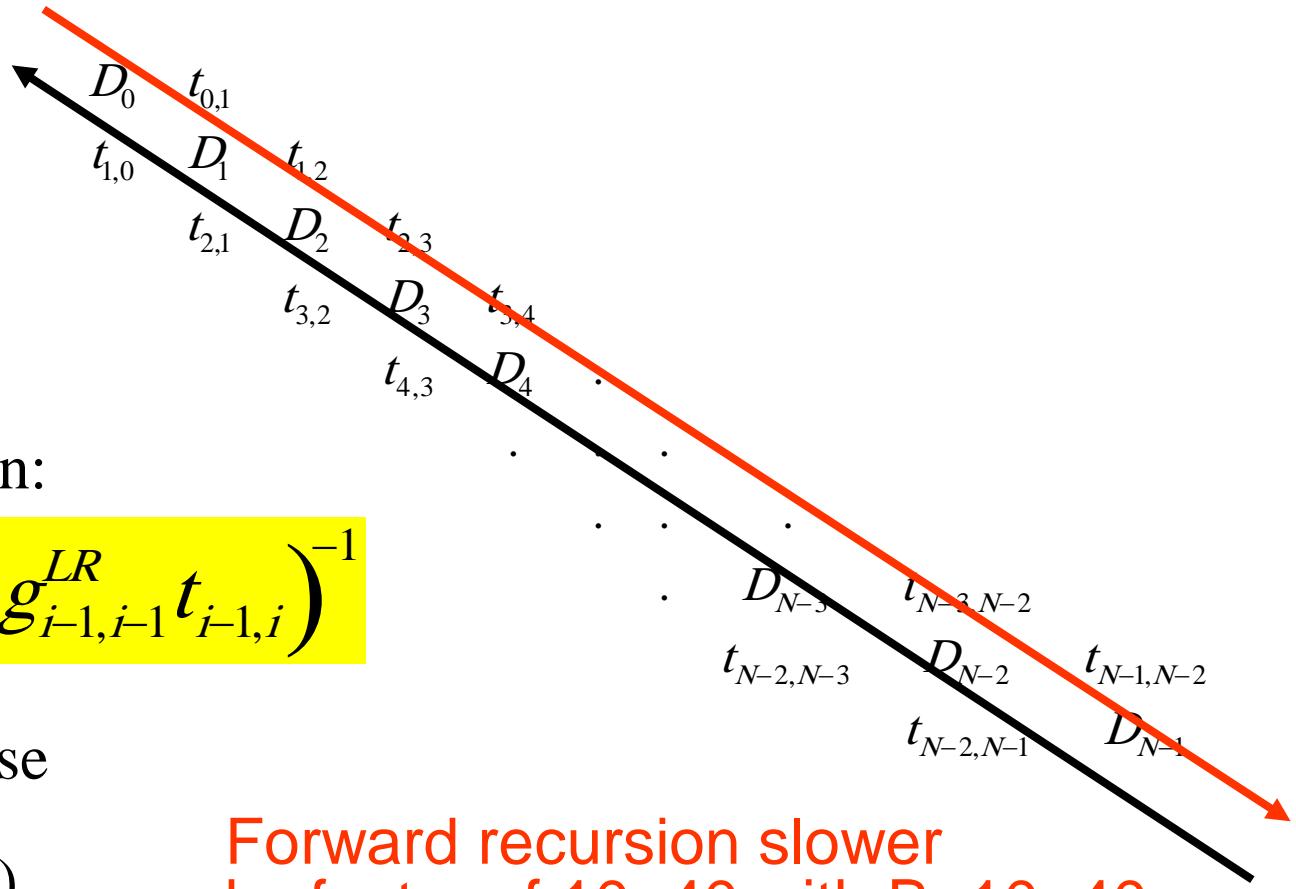
$$t_{N-2,N-1}$$

$$G_{N-1,N-1}^R$$

## Backward Recursion:

$G_{N-2,N-2}^R = g_{N-2,N-2}^{LR} \left( 1 + t_{N-2,N-1} G_{N-1,N-1}^R t_{N-1,N-2} g_{N-2,N-2}^{LR} \right)$   $G_{N-2,N-2}^R$  from  $G_{N-1,N-1}^R$  and  $g_{N-2,N-2}^{LR}$

$G_{i-1,i-1}^R = g_{i-1,i-1}^{LR} \left( 1 + t_{i-1,i} G_{i,i}^R t_{i,i-1} g_{i-1,i-1}^{LR} \right)$   $G_{i-1,i-1}^R$  from  $G_{i,i}^R$  and  $g_{i-1,i-1}^{LR}$



Forward Recursion:

$$g_{i,i}^{LR} = (D_i - t_{i,i-1} g_{i-1,i-1}^{LR} t_{i-1,i})^{-1}$$

Includes the inverse  
of the blocks:  
Scales as  $O(NxB^3)$

**Forward recursion slower  
by factor of 10~40 with  $B=10\sim40$   
Forward recursion is the bottle-neck!**

Backward Recursion:

$$G_{i-1,i-1}^R = g_{i-1,i-1}^{LR} (1 + t_{i-1,i} G_{i,i}^R t_{i,i-1} g_{i-1,i-1}^{LR})$$

Includes simple block  
multiplications:  
Scales as  $O(NxB^2)$

$$g_{i,i}^{LR} = \left( D_i - t_{i,i-1} g_{i-1,i-1}^{LR} t_{i-1,i} \right)^{-1} \quad \text{Left-connected set of equations}$$

$$G_{i-1,i-1}^R = g_{i-1,i-1}^{LR} \left( 1 + t_{i-1,i} G_{i,i}^R t_{i,i-1} g_{i-1,i-1}^{LR} \right)$$

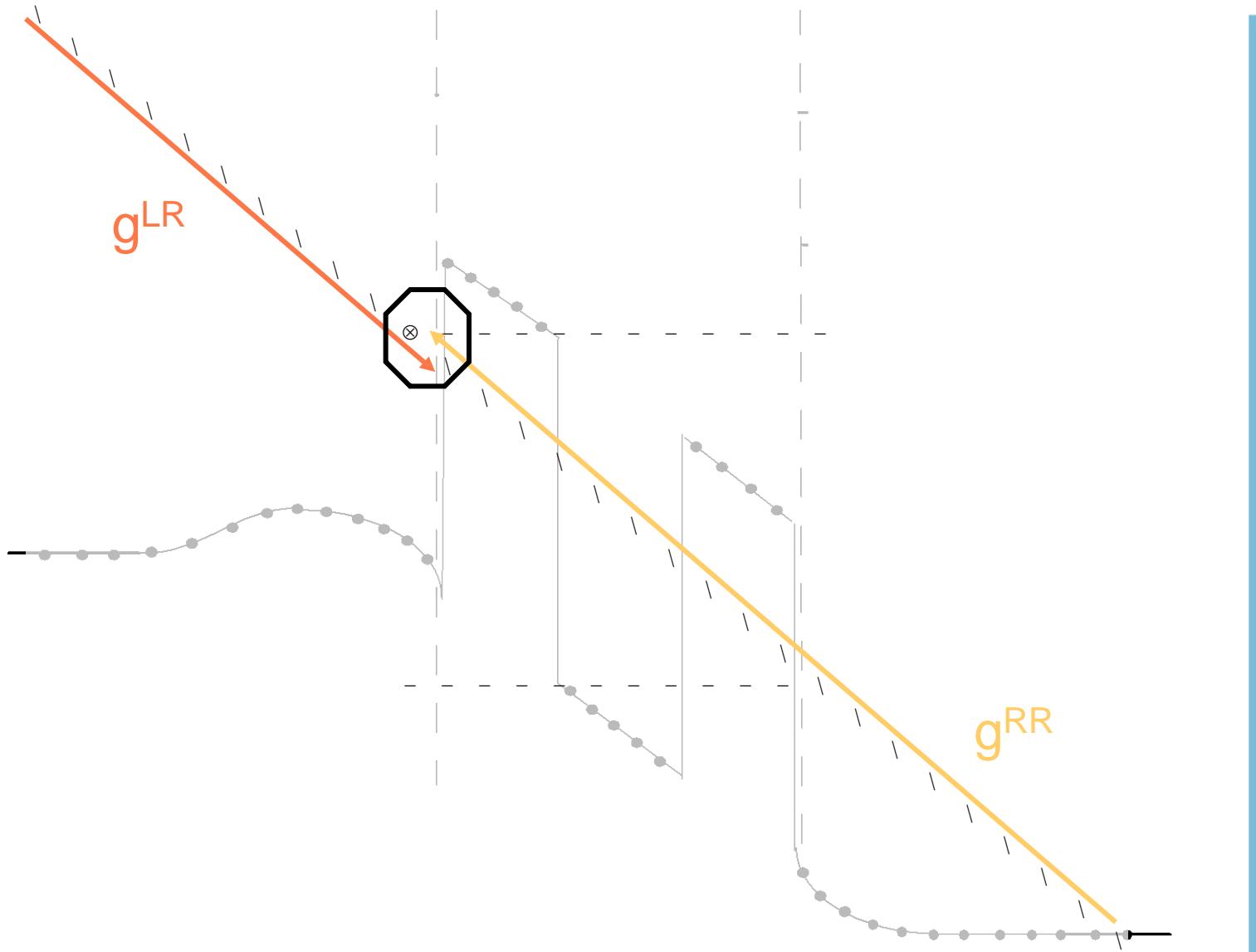
$$\left. \begin{array}{ccccccccc} & & & & & & & & \\ & t_{1,0} & D_1 & t_{1,2} & & & & & \\ & & \ddots & & & & & & \\ & t_{2,1} & D_2 & t_{2,3} & & & & & \\ & & \ddots & & & & & & \\ & t_{3,2} & D_3 & t_{3,4} & & & & & \\ & & \ddots & & & & & & \\ & t_{4,3} & D_4 & & \ddots & & & & \\ & & \ddots & & \ddots & & & & \\ & & & & \ddots & & & & \\ & & & & & D_{N-3} & t_{N-3,N-2} & & \\ & & & & & t_{N-2,N-3} & D_{N-2} & t_{N-1,N-2} & \\ & & & & & & \ddots & & \\ & & & & & & t_{N-2,N-1} & D_{N-1} & \end{array} \right\} G^R = 1$$

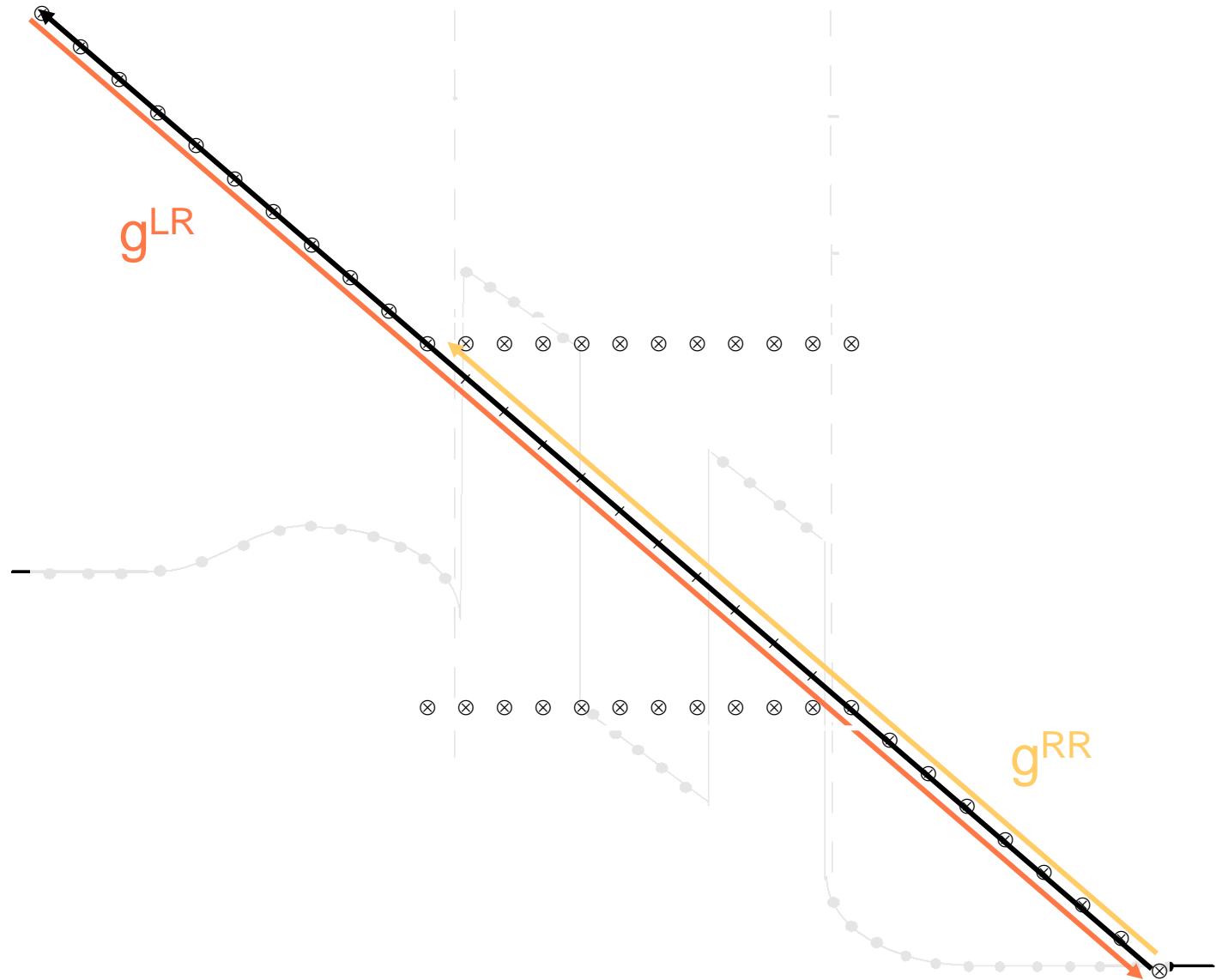
$$G_{i,i}^R = \left( 1 - g_{i,i}^{LR} t_{i,i+1} g_{i+1,i+1}^{RR} t_{i+1,i} \right)^{-1} g_{i,i}^{LR}$$

Right-connected set of equations

$$g_{i,i}^{RR} = \left( D_i - t_{i,i+1} g_{i+1,i+1}^{RR} t_{i+1,i} \right)^{-1}$$

$$G_{i+1,i+1}^R = g_{i+1,i+1}^{RR} \left( 1 + t_{i+1,i} G_{i,i}^R t_{i,i+1} g_{i+1,i+1}^{RR} \right)$$





$$G_{i,j}^R \Big|_{i < j} = G_{j,i}^R \Big|_{i < j} = -g_{i,i}^{LR} t_{i,i+1} G_{i+1,j}^R$$

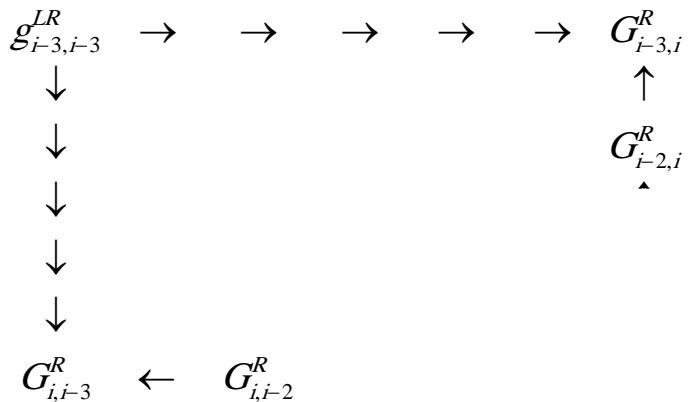
$$\begin{array}{ccc}
 g_{i-1,i-1}^{LR} & \rightarrow & G_{i-1,i}^R \\
 \downarrow & & \uparrow \\
 G_{i,i-1}^R & \leftarrow & G_{i,i}^R
 \end{array}$$

# General Expressions for Off-Diagonal Inverse Blocks

$$G_{i,j}^R \Big|_{i < j} = G_{j,i}^R \Big|_{i < j} = -g_{i,i}^{LR} t_{i,i+1} G_{i+1,j}^R$$

$$\begin{array}{ccccccc}
 g_{i-2,i-2}^{LR} & \rightarrow & \rightarrow & \rightarrow & G_{i-2,i}^R \\
 \downarrow & & & & \uparrow \\
 \downarrow & & & & G_{i-1,i}^R \\
 \downarrow & & & & \downarrow \\
 G_{i,i-2}^R & \leftarrow & G_{i,i-1}^R
 \end{array}$$

$$G_{i,j}^R \Big|_{i < j} = G_{j,i}^R \Big|_{i < j} = -g_{i,i}^{LR} t_{i,i+1} G_{i+1,j}^R$$



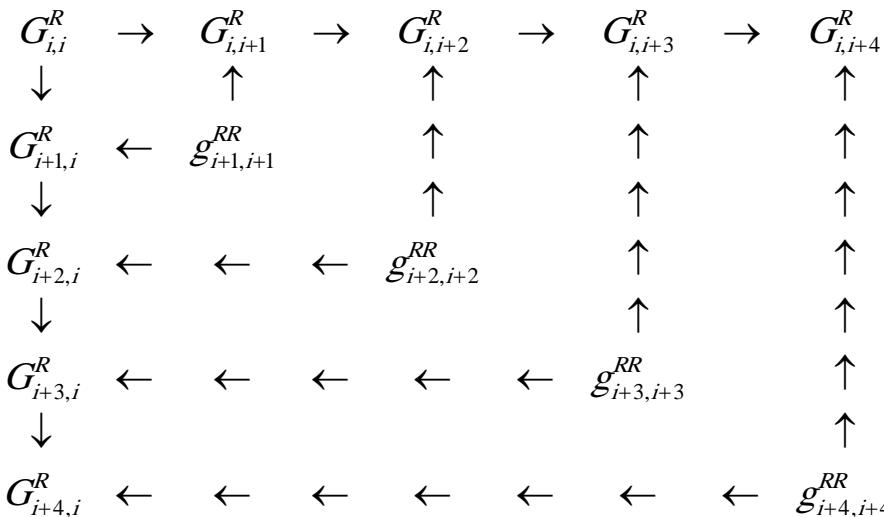
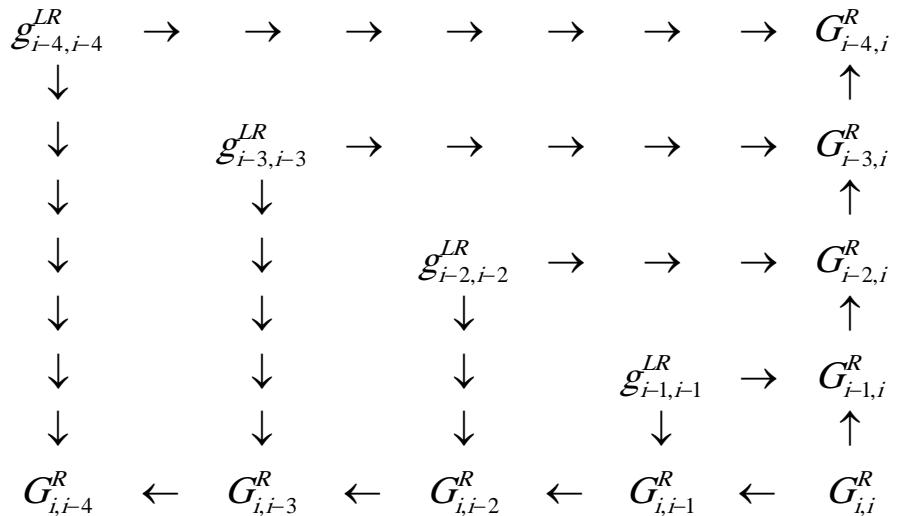
$$G_{i,j}^R \Big|_{i < j} = G_{j,i}^R \Big|_{i < j} = -g_{i,i}^{LR} t_{i,i+1} G_{i+1,j}^R$$

$$\begin{array}{cccccccccc}
 g_{i-4,i-4}^{LR} & \rightarrow & G_{i-4,i}^R \\
 \downarrow & & & & & & & & & \uparrow \\
 \downarrow & & & & & & & & & G_{i-3,i}^R \\
 \downarrow & & & & & & & & & \\
 \downarrow & & & & & & & & & \\
 \downarrow & & & & & & & & & \\
 \downarrow & & & & & & & & & \\
 \downarrow & & & & & & & & & \\
 G_{i,i-4}^R & \leftarrow & G_{i,i-3}^R
 \end{array}$$

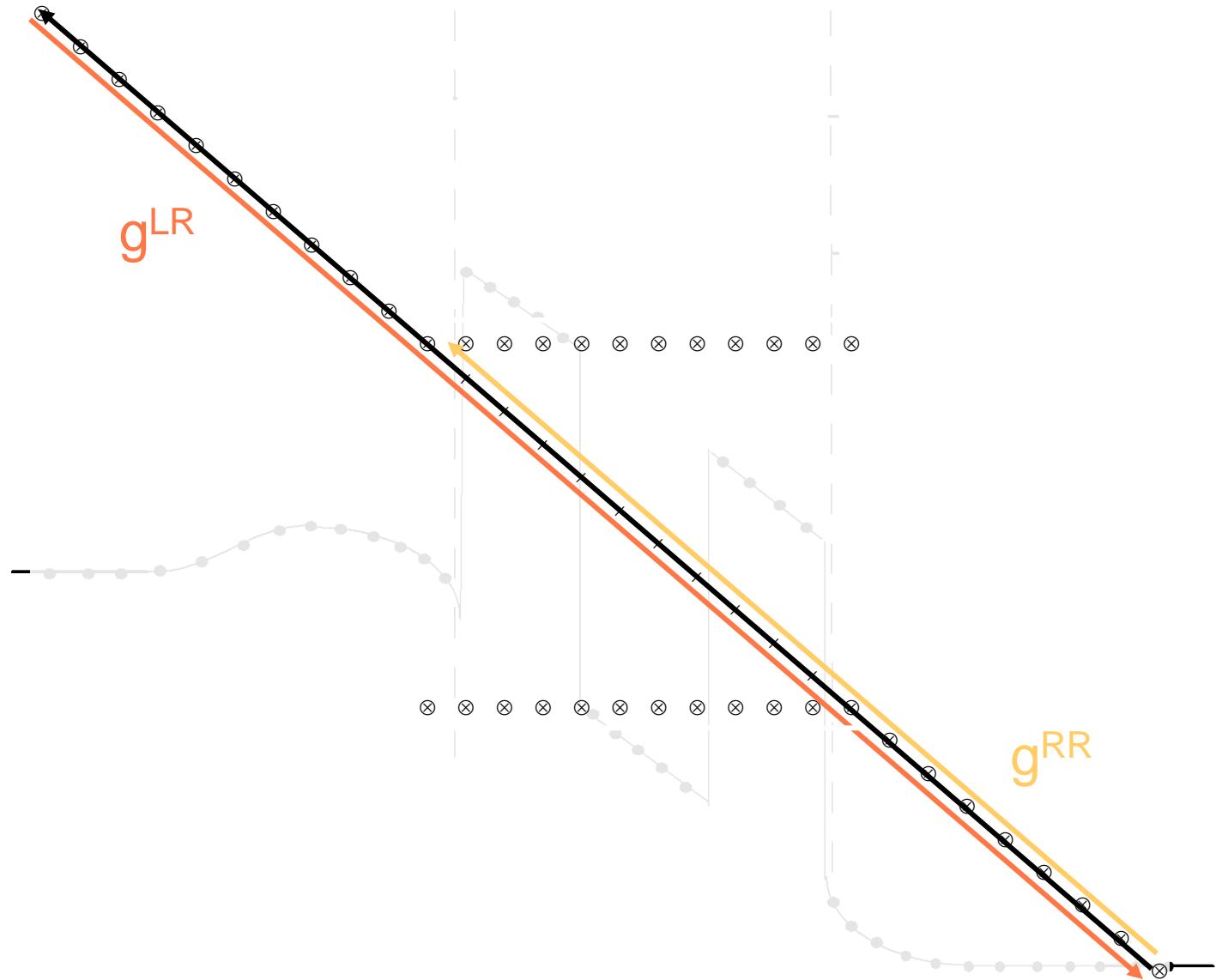
$$\boxed{G_{i,j}^R|_{i < j} = G_{j,i}^R|_{i < j} = -g_{i,i}^{LR} t_{i,i+1} G_{i+1,j}^R}$$

$$\begin{array}{ccccccccccccc}
 g_{i-4,i-4}^{LR} & \rightarrow & & G_{i-4,i}^R \\
 \downarrow & & & & & & & & & & & & & \uparrow \\
 \downarrow & & g_{i-3,i-3}^{LR} & \rightarrow & & G_{i-3,i}^R \\
 \downarrow & & \downarrow & & & & & & & & & & & \uparrow \\
 \downarrow & & \downarrow & & g_{i-2,i-2}^{LR} & \rightarrow & & \rightarrow & & \rightarrow & & & & G_{i-2,i}^R \\
 \downarrow & & \downarrow & & \downarrow & & & & & & & & & \uparrow \\
 \downarrow & & \downarrow & & \downarrow & & g_{i-1,i-1}^{LR} & \rightarrow & & & & & & G_{i-1,i}^R \\
 \downarrow & & \downarrow & & \downarrow & & \downarrow & & & & & & & \uparrow \\
 G_{i,i-4}^R & \leftarrow & G_{i,i-3}^R & \leftarrow & G_{i,i-2}^R & \leftarrow & G_{i,i-1}^R & \leftarrow & G_{i,i}^R & \leftarrow & & & & 
 \end{array}$$

$$G_{i,j}^R|_{i < j} = G_{j,i}^R|_{i < j} = -g_{i,i}^{LR} t_{i,i+1} G_{i+1,j}^R$$



$$G_{i,j}^R|_{i > j} = G_{j,i}^R|_{i > j} = -g_{i,i}^{RR} t_{i,i-1} G_{i-1,j}^R$$



- No incoherent scattering:

$$(E-H-\Sigma^R_{\text{bound}}) G^R = 1$$

- » No charge effects:

- ✓ Boundary conditions.
- ✓ Current on ONE site.

$$g^R_{\text{left},\text{left}} \quad g^R_{\text{right},\text{right}} \\ J \sim G^R_{i,i}$$

- » With charge effects:

- ✓ Boundary conditions.
- ✓ Current on one site.
- ✓ Charge throughout the
  - non-equilibrium device:  $N \sim \sum_j (G^R_{ij}) + \sum_j (G^R_{kj})$
  - device reservoirs:

$$g^R_{\text{left},\text{left}} \quad g^R_{\text{right},\text{right}} \\ J \sim G^R_{i,i} \\ N \sim G^R_{i,i}$$

Details in: Lake, Klimeck, Bowen and Jovanovic, J. of Appl. Phys. 81, 7845 (1997).

$$g_{i>0,i>0}^l = \left[ D_i - t_{i,i-1} g_{i-1,i-1}^l t_{i-1,i} \right]^{-1} \quad \text{with : } g_{0,0}^l = [D_0]^{-1}$$

$$g_{i < N-1, i < N-1}^r = \left[ D_i - t_{i,i+1} g_{i+1,i+1}^r t_{i+1,i} \right]^{-1} \quad \text{with : } g_{N-1,N-1}^r = [D_{N-1}]^{-1}$$

$$G_{i < N-1, i < N-1} = g_{i,i}^l \left( 1 + t_{i,i+1} G_{i+1,i+1} t_{i+1,i} g_{i,i}^l \right) \quad \text{with : } G_{N-1,N-1} = g_{N-1,N-1}^l$$

$$G_{i,i} = \left[ 1 - g_{i,i}^l t_{i,i+1} g_{i+1,i+1}^r t_{i+1,i} \right]^{-1} g_{i,i}^l$$

$$G_{i,j}|_{i < j} = G_{j,i}|_{i < j} = -g_{i,i}^l t_{i,i+1} G_{i+1,j}$$

$$G_{i,j}|_{i > j} = G_{j,i}|_{i > j} = -g_{i,i}^r t_{i,i-1} G_{i-1,j} .$$