Bigger and better: Large Scale NEGF Calculations and Coupling DFT with TB

Nick Rübner Papior



Outline



2 Non-equilibrium Green functions (TRANSIESTA)

- Block-Tri-Diagonal inversion
- Why pivoting matters?
- Scalability
- Optimizing the integration



OFT coupled to tight-binding – graphene • DFT \rightarrow TB

Motivation

1 Motivation

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DFT coupled to tight-binding – graphene
 ● DFT → TB

Motivation

Graphene







- Larger and larger devices
- Multiple electrodes
- Non-equilibrium effects

Non-equilibrium Green functions (TRANSIESTA)





Non-equilibrium Green function

Basic equations — and problems herein

Equations for calculating the density matrix

$$\mathbf{G}(z) = \left[z\mathbf{S} - \mathbf{H} - \sum_{e} \Sigma_{e}(z - \mu_{e}) \right]^{-1} \text{, with } z \equiv \epsilon + i\eta$$

$$\Gamma_{e}(z) = i \left(\Sigma_{e}(z - \mu_{e}) - \Sigma_{e}^{\dagger}(z - \mu_{e}) \right)$$

$$\rho(z) \sim -\int \left[\mathbf{G}(z) - \mathbf{G}^{\dagger}(z) \right] n_{F,e} + \int \mathbf{G}(z) \Gamma_{e'}(z) \mathbf{G}^{\dagger}(z) [n_{F,e'} - n_{F,e}] dz$$



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Sparse elements

- Sparse inversion techniques, MUMPS, PEXSI, ...
- Sparsity depends on basis set



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Dense column matrix multiplications

- Sparse inversion techniques are less optimal
- Dense matrix operations may be more efficient \rightarrow Block-Tri-Diagonal (BTD)

Inversion — Block-Tri-Diagonal

Green function

Utilise sparsity of Hamiltonian

- Reduce complexity using zeroes
- Same as the recursive Green function algorithm



Reuter *et.al.*: 10.1088/1749-4699/5/1/014009 Papior *et.al.*: 10.1016/j.cpc.2016.09.022

Enforcing BTD — going quasi 1D

Pivoting matrix elements, order from dis-order

- 2,400 atoms
- 21,600 orbitals



Enforcing BTD — going quasi 1D

Pivoting matrix elements, order from dis-order

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Speedup and scalability





Speedup and scalability



Brandbyge *et.al.*: 10.1103/PhysRevB.65.165401 Papior *et.al.*: 10.1016/j.cpc.2016.09.022

Currently known investigated systems



Brandimarte et.al.: 10.1063/1.4974895, Obesteiner et.al.: 10.1021/acs.nanolett.7b03066

Energy contour

 $\bullet\,$ Integration in the complex plane for the equilibrium contour $G-G^{\dagger}$



Energy contour

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- Gaussian quadrature have more points close to the integration boundaries



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k-points on

- $\bullet\,$ Bias window calculation $G\Gamma G^{\dagger}$
- Only states close to the reference energy are important!





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 $\mathsf{DFT}\to\mathsf{TB}$



- Current problems involve a model-tip coupling via Γ
- For complex chemical defects and/or complex electrode attachments, tight-binding is *not* accurate enough

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Gaetano Calogero

- Calculate the self-energy from the tip-electrode region
- Propagate the self-energy onto the red atoms
- Cut the self-energies to the parameterized orbitals

 $\mathsf{DFT}\to\mathsf{TB}$

DFT

Two DFT calculations are carried out:

- Pristine graphene calculation from which TB parameters are extracted.
- Calculation of a defected region surrounded by pristine (in every sense) graphene. The pristine graphene region must be big enough to screen the "defected" region.

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Tight-binding

From pristine DFT calculation extract the non-orthogonal parameters up to a user-specified range. These parameters are used to construct a non-orthogonal tight-binding model of pristine graphene to a user-defined size. Next, any region of the system may be replaced by the self-energy describing local defects.

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• Selecting the parameters is done using the orbitals that have all the weight in the energy range specified.

• It is crude, but it works!

Gold STM tip



Gold STM tip



Standardized method

More than one region of defects



Two-tip structure by inserting the same tip in two different places. Bond-currents from the left tip are seen.

Co-workers and collaborators

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