

How to Use NEGF Matrix Formulas: Step-by-Step Tutorial in Pictures

Branislav K. Nikolić

Department of Physics & Astronomy, University of Delaware, Newark, DE 19716, U.S.A.

<https://wiki.physics.udel.edu/phys824>

The screenshot shows the 'Main Page' of the PHYS 824: Introduction to Nanophysics course. The page is titled 'PHYS 824: Introduction to Nanophysics' and includes a brief description of the course. It features a sidebar with navigation links, a search bar, and a list of course topics. The main content area includes a diagram of a nanoscale device and a list of topics. The right sidebar contains news, lecture progress, quick links, and a course motto.

PHYS 824
Introduction to Nanophysics

Main Page

PHYS 824: Introduction to Nanophysics

The 12-hour version of the course was offered at the National Taiwan University in March 2010
The 15-hour version of the course was offered at the University of Belgrade, Serbia in June 2010

Instructor: UD Physics & Astronomy - Teaching Web

Course Topics

The course provides **hands-on experience** (including one hour of Computer Lab per week) for graduate students in sciences (physics, chemistry, applied mathematics) and engineering (electrical, chemical, materials) to analyze electronic structure and transport properties of basic classes of nanostructures explored at the current research frontiers

Nanostructures in equilibrium: graphene and other layered materials, carbon nanotubes, topological insulators, magnetic multilayers.

Nanostructure out of equilibrium: conductance quantization, quantum interference, spin-dependent tunneling, spin-transfer torque, I-V curves

Theoretical techniques: elements of density functional theory (DFT), Boltzmann transport equation, spin and charge diffusion equations, Landauer-Büttiker scattering formalism, nonequilibrium Green function techniques

Experimental techniques: scanning tunneling and atomic force microscopy

Applications: nanoelectronics, spintronics, thermoelectrics

News

- Fall 2016 course will start on Tuesday, August 30.
- For the first time, students have an option to select between research and conventional track for getting a grade in the course.

Lecture in Progress

- Lecture 1: What is nanophysics: Introduction to course topics

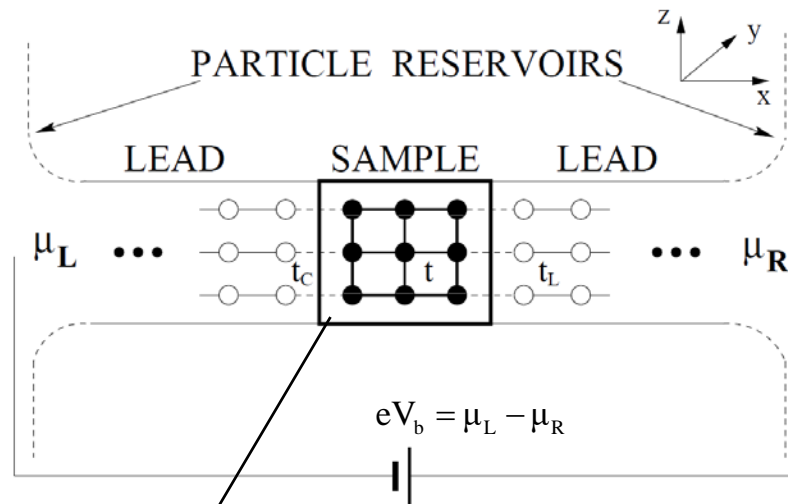
Quick Links

- KWANT package
- GPW package
- Video lectures on AFM and STM from nanohub.org
- Spotlighting Exceptional Research in Nanophysics
- DPA Condensed Matter & Nanophysics seminar series

Course Motto

- In teaching, writing, and research, there is no greater clarifier than a well-chosen example
- Formalism should not be introduced for its own sake, but only when it is needed for some particular

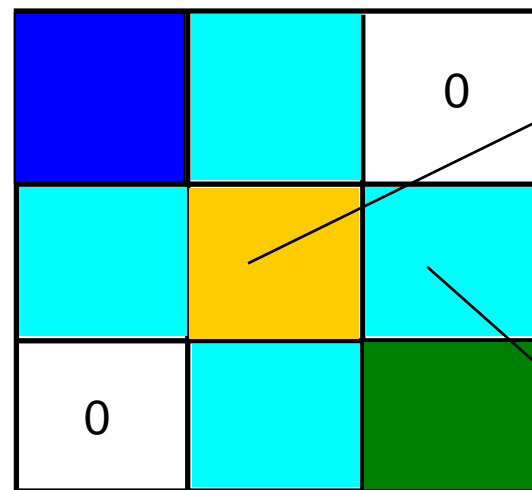
Step 1: Construct Matrix Representation of the Tight-Binding Hamiltonian of Central Region



3x3 lattice of atoms in the central region

9x9 Hamiltonian matrix

	I	II	III
I	●	●	●
II	●	●	●
III	●	●	●



3x3 submatrix describing second row of atoms

3x3 submatrix describing hoppings from third to second row of atoms

Step 2: Construct Self-Energy Matrices for the Left and the Right Semi-Infinite Lead

9x9 self-energy matrix for the left electrode

	0	0
0	0	0
0	0	0

→ 3x3 submatrix of non-zero elements which is returned by the Function `self_energy.m`

9x9 self-energy matrix for the right electrode

0	0	0
0	0	0
0	0	

Since self-energies are summed with the Hamiltonian before inversion to get the Green function of an open system, they MUST be defined on the same Hilbert space of 9 orbitals

```

H(1:3,1:3)=H1;
H(7:9,7:9)=H3;
for energy=-4:0.02:4
    sigma=self_energy(3,1,energy,t_lead,t_couple);
    H(1:3,1:3)= H(1:3,1:3)+sigma;
    H(7:9,7:9)= H(7:9,7:9)+sigma;
    Gr=inv(energy*eye(Hsize,Hsize)-H);
    
```

MATLAB

This self-energy (i.e., its non-zero 3x3 block returned by the function) is added onto the corners (representing edge layers of the 3x3 sample) of the ORIGINAL Hamiltonian recorded outside of the loop

Step 3: Construct Retarded Green Function for an Open Quantum System

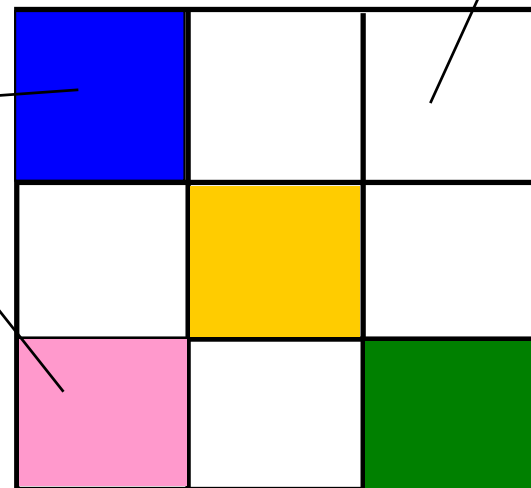
9x9 retarded Green function matrix

This 3x3 submatrix is composed of quantum-mechanical probability amplitudes for electron to propagate between I and ||| row of atoms. This, it must be related to the scattering matrix concept in the Landauer formalism (which contains probability amplitude to propagate from a conducting channel in left led to a conducting channel in the right lead)

	I	II	III
3	●	●	●
2	●	●	●
1	●	●	●

This 3x3 submatrix is composed of quantum-mechanical probability amplitudes for electron to propagate between ||| and I row of atoms. For example, matrix element G_{29} gives probability amplitude to propagate from atom 9 to atom 2.

This 3x3 submatrix allows us to compute the local density of states on each atom from row | using $-\text{Im } G / \pi$. The total density of states is then obtained by summing all elements of on the diagonal of $-\text{Im } G / \pi$



Step 4: Compute Transmission Function Using NEGF-based Implementation of the Landauer Formula

$$T(E) = \text{Tr} \left(\begin{array}{c} \Gamma_R \quad G \quad \Gamma_L \quad G^\dagger \\ \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \square \\ \hline \square & \square & \textcolor{red}{\square} \\ \hline \end{array} \quad \begin{array}{|c|c|c|} \hline \textcolor{blue}{\square} & \square & \square \\ \hline \square & \textcolor{yellow}{\square} & \square \\ \hline \textcolor{pink}{\square} & \square & \textcolor{green}{\square} \\ \hline \end{array} \quad \begin{array}{|c|c|c|} \hline \textcolor{red}{\square} & \square & \square \\ \hline \square & \square & \square \\ \hline \square & \square & \square \\ \hline \end{array} \quad \begin{array}{|c|c|c|} \hline \textcolor{blue}{\square} & \square & \square \\ \hline \square & \textcolor{yellow}{\square} & \square \\ \hline \textcolor{pink}{\square} & \square & \textcolor{green}{\square} \\ \hline \end{array} \end{array} \right)$$

One can compute the transmission function by either of these two formulas. However, the top one, which is a brute force transfer from paper-pencil into computer, requires many more matrix multiplication operations. Instead, one can check by paper-pencil that the bottom one is equivalent to it and substantially speed up computation. Furthermore, this means that only the 3x3 submatrix of the total Green function, which connects atoms on the edges of the central region (where the leads are attached) should be computed by partially inverting the open system Hamiltonian matrix.

$$T(E) = \text{Tr} \left(\begin{array}{c} \text{non-zero submatrix of } \Gamma_R \quad \text{submatrix of } G \quad \text{non-zero submatrix of } \Gamma_L \quad \text{non-zero submatrix of } G^\dagger \\ \begin{array}{|c|} \hline \textcolor{red}{\square} \\ \hline \end{array} \quad \begin{array}{|c|} \hline \textcolor{pink}{\square} \\ \hline \end{array} \quad \begin{array}{|c|} \hline \textcolor{red}{\square} \\ \hline \end{array} \quad \begin{array}{|c|} \hline \textcolor{pink}{\square} \\ \hline \end{array} \end{array} \right)$$