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

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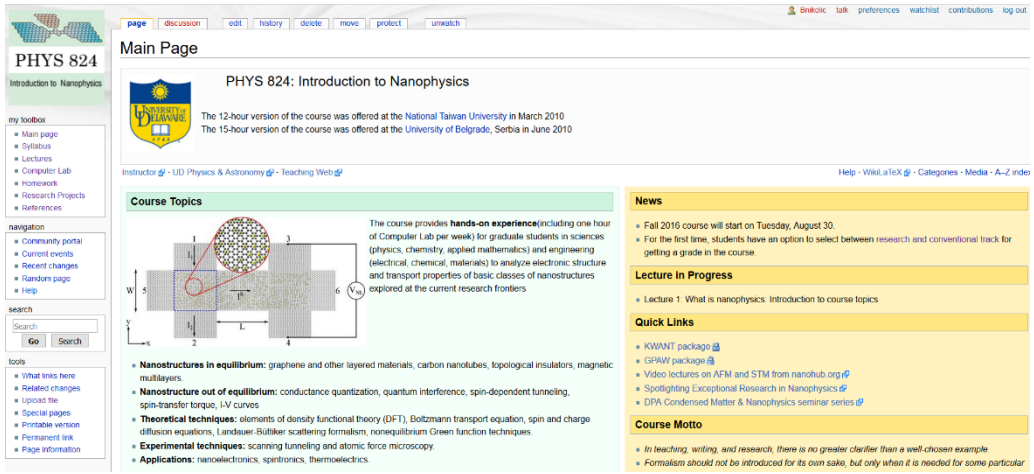
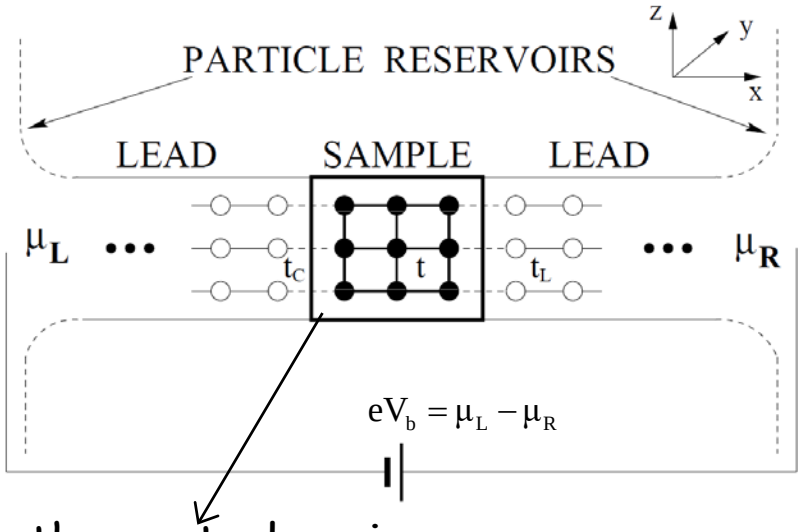
https://wiki.physics.udel.edu/phys824

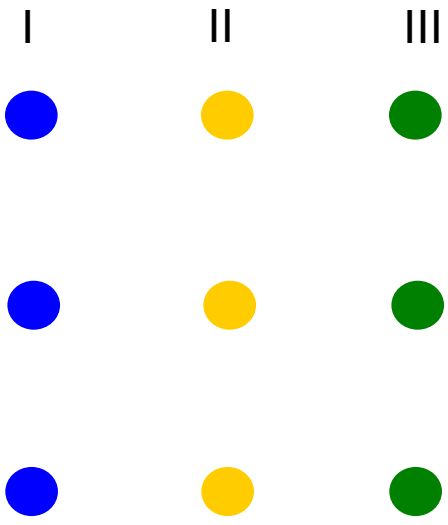


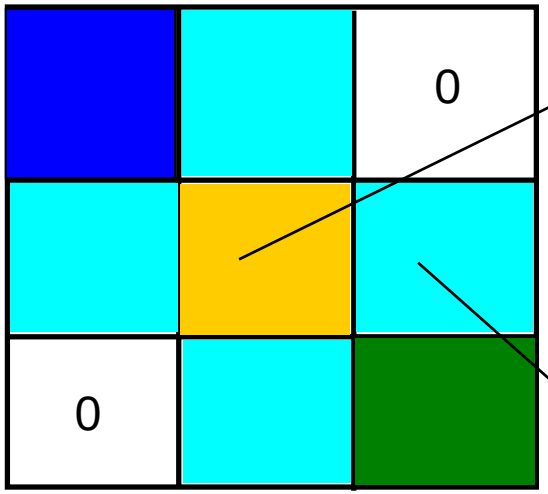
Step 1: Construct Matrix Representation of the Tight-Binding Hamiltonian of Central Region



3x3 lattice of atoms in the central region

9x9 Hamiltonian matrix





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

MATLAB

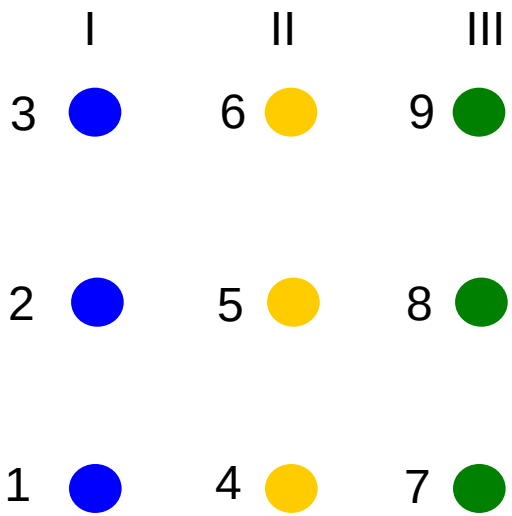
```
H(1:3,1:3)=H1;
H(7:9,7:9)=H3;
for energy=-4:0.02:4
    sigma=self_energy(3,1,energy,t_lead,t_couple);
    H(1:3,1:3)= H(1:3,1:3)+sigma;
    H(7:9,7:9)= H(7:9,7:9)+sigma;
    Gr=inv(energy*eye(Hsize,Hsize)-H);
```

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 Hamiltonan recorded outside of the loop

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

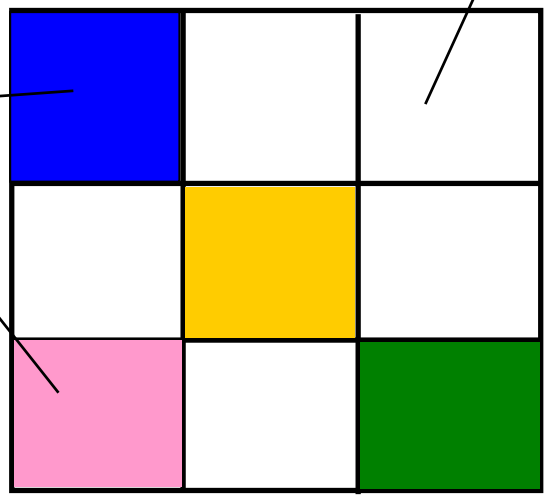
9x9 retarded Green function matrix

This 3x3 submatrix is composed of quantum-mechanical probability amplitudes for electron to propagate between I and III 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)



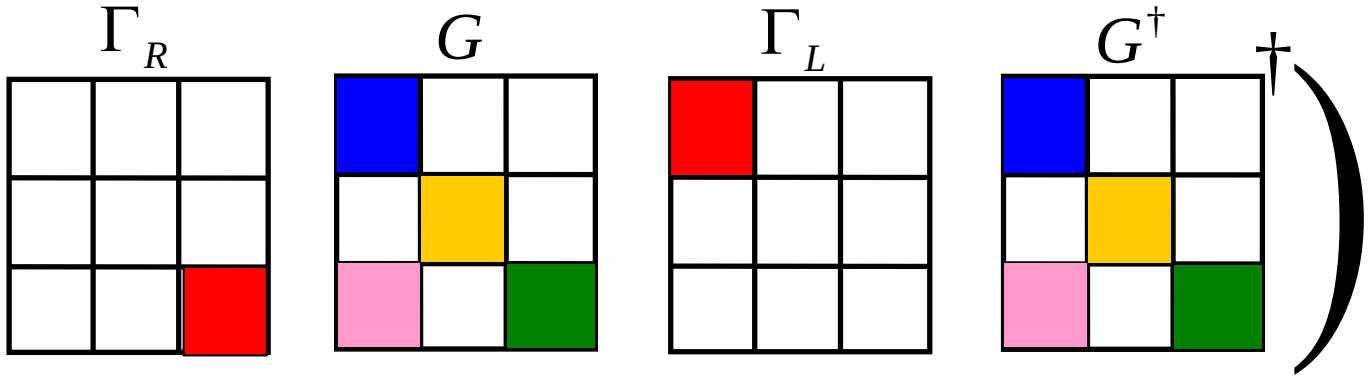
This 3x3 submatrix is composed of quantum-mechanical probability amplitudes for electron to propagate between III and I row of atoms. For example, matrix element G_{29} gives probability amplitude to propagate from atom 9 to atom 2.

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



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

$$T(E) = \mathrm{Tr}\left(\Gamma_R \; G \; \Gamma_L \; G^{\dagger} \right)^{\dagger}$$



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.

$$T(E) = \mathrm{Tr}\left(\Gamma_R \; G_{|||,|} \; \Gamma_L \; \right)^{\dagger}$$

non-zero submatrix of Γ_R | submatrix of G $G_{|||,|}$ | non-zero submatrix of Γ_L