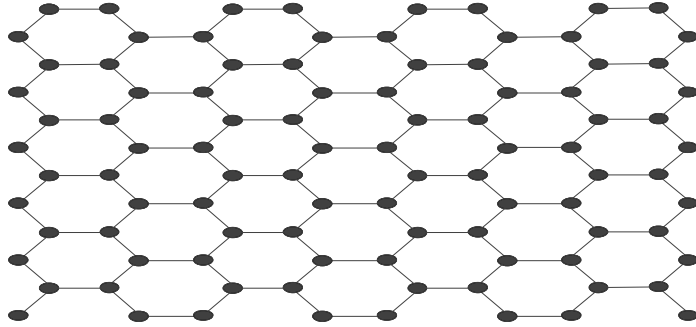I am a Ph.D. Student. I want to obtain the Local Density of States (LDOS) and then electron density of a 12-AGNR using NEGF.

My algorithm to implement LDOS in MATLAB is as follow:

$$\beta_1 = \begin{bmatrix} -3 & 0 & 0 & 0 & 0 & 0 \\ 0 & -3 & 0 & 0 & 0 & 0 \\ 0 & 0 & -3 & 0 & 0 & 0 \\ 0 & 0 & 0 & -3 & 0 & 0 \\ 0 & 0 & 0 & 0 & -3 & 0 \\ 0 & 0 & 0 & 0 & 0 & -3 \end{bmatrix}, \quad \beta_2 = \begin{bmatrix} -3 & 0 & 0 & 0 & 0 & 0 \\ -3 & -3 & 0 & 0 & 0 & 0 \\ 0 & -3 & -3 & 0 & 0 & 0 \\ 0 & 0 & -3 & -3 & 0 & 0 \\ 0 & 0 & 0 & -3 & -3 & 0 \\ 0 & 0 & 0 & 0 & -3 & -3 \end{bmatrix}$$

$$H = \begin{bmatrix} [0]_{6*6} & \beta_2 & & & & \\ \beta_2' & [0]_{6*6} & \beta_1 & & & \\ & \beta_1 & [0]_{6*6} & \beta_2' & & \\ & & \beta_2 & [0]_{6*6} & \beta_1 & \\ & & & \beta_1 & [0]_{6*6} & \cdots \\ & & & & \cdots & \cdots \end{bmatrix}$$

Then for each E, I calculate gs and gd (S/D surface green func.) using recursive algorithm as follows:

```
    G1_old        = inv(E*eye(nA_T)-alfa{1});
    G2_old        = inv(E*eye(nA_T)-alfa{2});
    while diff1 >errmax || diff2>errmax
        G1_new        = inv((EE*eye(nA_T))-alfa{1}-(beta2'*G2_old*beta2));
        G2_new        = inv((EE*eye(nA_T))-alfa{2}-(beta1'*G1_old*beta1));
        diff1         = (sum(sum(abs(G1_new-G1_old))))/(sum(sum(abs(G1_new+G1_old))));
        diff2         = (sum(sum(abs(G2_new-G2_old))))/(sum(sum(abs(G2_new+G2_old))));
        G1_old        = G1_new;
        G2_old        = G2_new;
    End
```

and the same algorithm is used to calculate gd.

Then I obtain:

```
    Sigma_11=beta1*g1*beta1';
    sigma1=zeros(N_Atoms);
    sigma1(1:nA_T ,   1:nA_T)=Sigma_11;

    Sigma_nn=beta1*g1*beta1';
    sigma2=zeros(N_Atoms);
    sigma2(N_Atoms-nA_T+1:N_Atoms ,   N_Atoms-nA_T+1:N_Atoms)=Sigma_nn;

    gamma1 = 1i*(sigma1-sigma1');
    gamma2 = 1i*(sigma2-sigma2');
    Green_inv = (EE*eye(N_Atoms))-H-sigma1-sigma2;
    G = inv(Green_inv);

T (jj)= real(trace(gamma1*G*gamma2*G'));

LDOS_S=G*gamma1*G';   % The Source Local Density of States (LDOS)
```

But LDOS calculated by this method seems to be false, because **electron density do not remain constant against width of GNR.**

Please guide me