ECE 659   Spring '09
HW #5 Due Friday March 27, 2009 in class

Conductance quantization of Carbon Nanotube(CNT) and Graphene Nanoribbon(GNR)

1. **Consider uniform GNR structure in figure (Armchair edge GNR) .**

(a) Set up the Hamiltonian for GNR structure. You should first construct two block matrices α and β as shown in the figure below. The number of carbon atoms along the zigzag line(defined as in the figure) is 50(=N). In other words, there are 25 α_i's inside α matrix. To obtain the contact self-energies, use iterative solution to calculate surface green function which is given by $g_{n+1} = [EI - \alpha - \beta g_n \beta^+]^{-1}$. Plot the transmission T(E) versus energy E (-0.6 < E < +0.6 eV), assuming t_0=-2.5eV (P_z orbital coupling energy between two adjacent carbon atoms). The coupling energy between carbon atoms is given by this t_0 value and on-site energy is assumed to be zero.

(b) The transmission should show a series of steps at different values of the energy as new modes start conducting. Compare the energies at which these steps occur with the analytical values for the transverse mode energies calculated using the following equation. ($|t_0||1 - 2\cos(ka)|$ where $ka = \dfrac{\pi q}{(N+1)}$ and q=1,2,3,…)

(c) Plot the bandstructure for GNR above. Compare the energy points where new subbands start with the energies where the transmission step occur from the previous result.
To calculate E-k relation with given α and β, find eigenvalues of h(k)= eig(α+βexp[ikd] +β^+exp[-ikd]) and plot as a function of k where d is a distance between unit cells(α).

2. Consider uniform CNT structure in figure (Zigzag CNT).

(a),(b),(c) Do the same calculation for CNT structure using periodic boundary condition as indicated in figure.
(for problem (b), use $|t_0||1 - 2\cos(ka)|$ where $ka = \dfrac{2\pi q}{N}$ and q= 0,±1, ±2, ±3,…)

width

transport

GNR structure

zigzag line

t_0

α   α

β

$\dots$ α β^+ α β α $\dots$
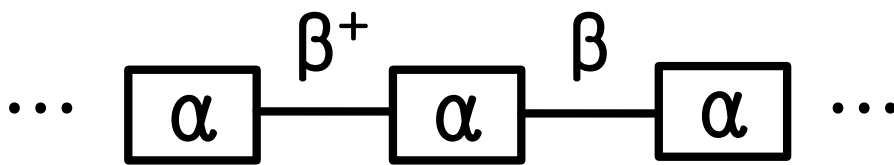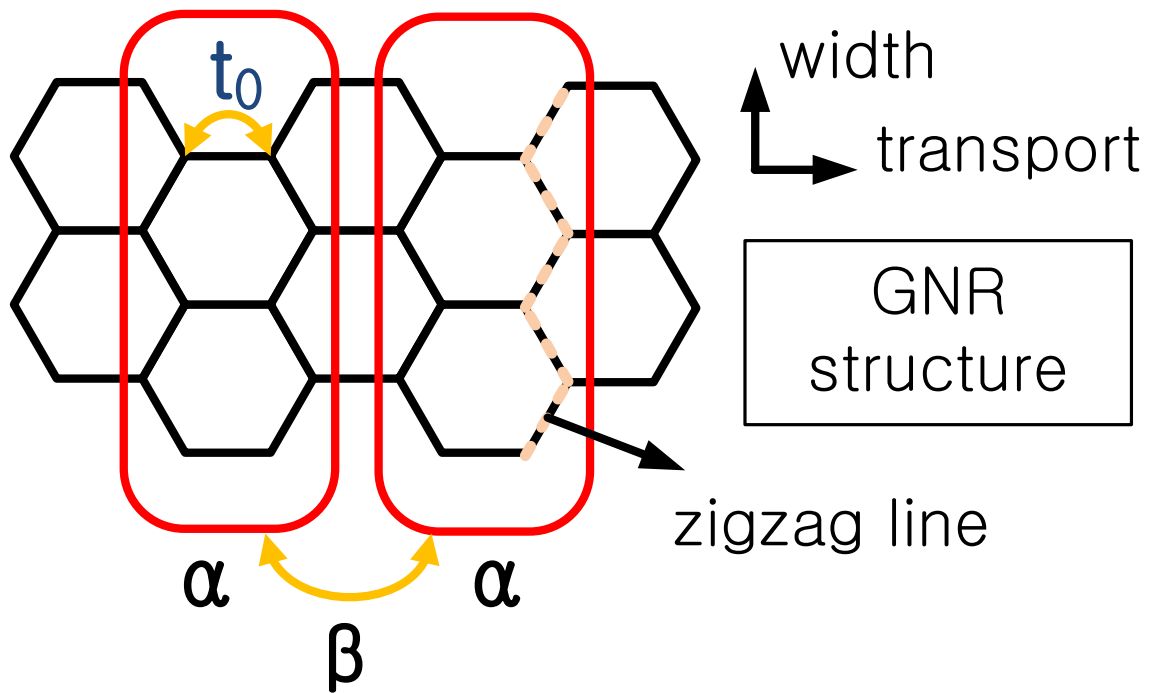
For example, you can construct Hamiltonian matrix using the following convention.

● : carbon atom

α_1

α_2

α_3

α

β
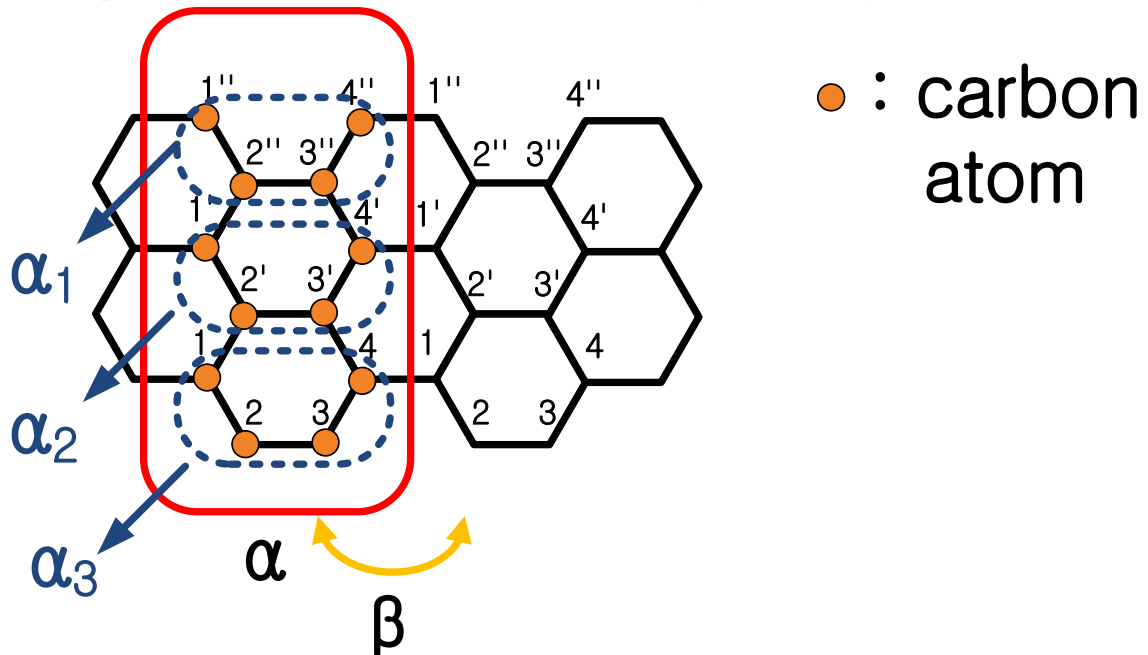
In CNT structure, $\alpha_{N+1} = \alpha_1$ which is a periodic boundary condition.

$$\alpha = \begin{bmatrix} \alpha_1 & \beta_w & 0 & 0 \\ \beta_w{}' & \alpha_2 & \beta_w & 0 \\ 0 & \beta_w{}' & \alpha_3 & \beta_w \\ 0 & 0 & \beta_w{}' & \ddots \end{bmatrix}$$

where $\alpha_1 =$

atom index	1	2	3	4
1	0	t_0	0	0
2	t_0	0	t_0	0
3	0	t_0	0	t_0
4	0	0	t_0	0

and $\beta_w =$

	1'	2'	3'	4'
1	0	0	0	0
2	t_0	0	0	0
3	0	0	0	t_0
4	0	0	0	0

In addition, the whole Hamiltonian matrix will be given by this.

$$H = \begin{bmatrix} \alpha & \beta & 0 & 0 \\ \beta' & \alpha & \beta & 0 \\ 0 & \beta' & \alpha & \beta \\ 0 & 0 & \beta' & \ddots \end{bmatrix}$$

where $\beta = \begin{bmatrix} \beta_L & 0 & 0 & 0 \\ 0 & \beta_L & 0 & 0 \\ 0 & 0 & \beta_L & 0 \\ 0 & 0 & 0 & \ddots \end{bmatrix}$ and $\beta_L = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ t_0 & 0 & 0 & 0 \end{bmatrix}$

These are the plots that you are supposed to get.