Physics of atoms and molecules

Assignment 1

A. Plot the density of eigen states (D(E)) of an $\mathrm{N}\times N$ matrix H with:

$\mathrm{H}_{i,i} = E_0$ for $i = 1, N; H_{i,i+1} = \beta$ for $i = 1, N-1; H_{i-1,i} = \beta$ for $i = 2, N$.

Choose E_0 to be any number and $\mid \beta \mid$ to be typically less than $\mid E_0 \mid$ as is generally the case in molecules.

Vary β and see how D(E) evolves. Plot D(E) for increasing N. Reflect on the width of the band as it converges with increasing N for any particular set of E_0, β.

B. Consider H with:

$\mathrm{H}_{i,i} = E_1$ for odd i ; $H_{i,i} = E_2$ for even i $H_{i,i+1} = \beta$ for $i = 1, N-1; H_{i-1,i} = \beta$ for $i = 2, N$.

Choose $\mid \beta \mid$ less than $\mid E_1 \mid$ and $\mid E_2 \mid$.

Vary β with respect to $\mid E_1 - E_2 \mid$ and see how the D(E) and gap between the bands changes. Plot D(E) for increasing N. Reflect on the width of the bands and the gap as it converges with increasing N for any particular set of E_1, E_2, β.

In this assignment you are actually plotting density of states of chains of mono-atomic (A) and diatomic (B) molecules.

To plot the density of eigen values see maximum and minimum eigen value E_{max} and E_{min} and divide their interval into n sub-interval and count the number of eigen values within each sub-interval. This is basically a histogram.

C. Now in both A and B put $\mathrm{H}_{1,N} = H_{N,1} = \beta$ and see how your plots changes.
With this the chain becomes a ring.

Upload pdf files with your codes and plots at assignment_1@10.0.6.49 using scp.
Password: phys2018_1
Name you assignment clearly with your name.