Fida Salim

1811065

**PLOTTING DENSITY OF EIGENSTATES**

The density of eigenstates for a mono-atomic chain of molecules were plotted. For this, an NxN matrix was created and their eigenvalues were obtained. For plotting, the matrix is tridiagonal with E0 as diagonal elements and as off-diagonal elements.

Q1. Mono-atomic molecule

The different plots were made by changing the parameters N, E0 and

N values were taken as 10,50,146,347,568,750,1023,1576,2000. As N was increased, the width of the bands is increased as well as the density of the states also increased. As N increased the whole band turns out to be a continuous strip rather than discrete. By changing the E0 as -5, -10, -15, -20 for a fixed = 1 and changing as 0.5,1,2,3 for fixed E0 = -10, the plots were created. For fixed E0, changing increased the broadness of the eigenstates range. For E0 = -10, had the eigenstate’s range from -11 to -9, whereas had eigenstate’s range from -12 to -8. On varying E0 with fixed the density of states remained the same.

Q2 Diatomic molecule

The different plots were made by changing the parameters N, |E1 – E2| and

N values were taken as 10,50,146,347,568,750,1023,1576,2000. As N was increased, the width of the bands increased as well as the density of the states also increased. E1 = -10 was fixed but E2 was varied as -9,-6,-8,-7,-5. For a fixed E2 = -6, and varying from 0.5,1,2,3, the plots were created. It was found the energy gap was fixed for every But the range of eigenstates became broader as increased. When |E1 – E2| was increased on fixed , the energy gap also increased. The density of the states was also increasing as |E1 – E2| increased.

Q3.

The last and the first atom of the monoatomic and diatomic molecule is allowed to interact. For the corner entries of the matrix is made non-zero and plotted. The plot did not seem different from the former Q1 and Q2. Since the first and last atom is allowed to interact, the chain of atom is supposed to become a ring.