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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 E_0 as diagonal elements and β as off-diagonal elements.

Q1. Mono-atomic molecule
The different plots were made by changing the parameters N, E_0 and β.
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 E_0 as -5, -10, -15, -20 for a fixed β = 1 and changing β as 0.5,1,2,3 for fixed E_0 = -10, the plots were created. For fixed E_0, changing β increased the broadness of the eigenstates range. For E_0 = -10, $\beta = 0.5$ had the eigenstate's range from -11 to -9, whereas $\beta = 1$ had eigenstate's range from -12 to -8. On varying E_0 with fixed $\beta = 1$, the density of states remained the same.

Q2 Diatomic molecule
The different plots were made by changing the parameters N, $|E_1 - E_2|$ and β.
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. E_1 = -10 was fixed but E_2 was varied as -9,-6,-8,-7,-5. For a fixed E_2 = -6, and varying β from 0.5,1,2,3, the plots were created. It was found the energy gap was fixed for every β. But the range of eigenstates became broader as β increased. When $|E_1 - E_2|$ was increased on fixed β, the energy gap also increased. The density of the states was also increasing as $|E_1 - E_2|$ 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.