

Assignment 1 Conclusions

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For monoatomic chain

We see in the plotted distributions that the density is maximum for extremes, i.e. the max and the minimum eigenvalues. By increasing N we can see that the band width increases and converges at a certain value for given E and $Beta$. By varying $Beta$ we see that the band width increases.

For Monoatomic ring

We see that the band width oscillates but effectively increases and eventually converges with N , same as chains, we can see the density is max for extremes. With $Beta$, the bandwidth increases in a similar fashion as with the chain.

For Diatomic chain

For the diatomic case, we see two different bands as expected, in each band the density is highest for its lowest and highest eigenvalue. We can also see that with N the bandwidth increases and converges. The gap between the two bands also increases and converges. With $Beta$, bandwidth increases, however no appreciable change in the gap is observed.

For Diatomic ring

Bandwidth increases with $beta$ and N and eventually converges similar to monoatomic rings. The nature of increasing bandwidth is similar to that in monoatomic chain as observed for different plots analytically.