ASSIGNMENT 1
Physics of Atoms and Molecules

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I. MONOATOMIC MOLECULES

```

import numpy as np
import matplotlib.pyplot as plt
import math
#Creating the matrix
A = int(input("Enter the diagonal value:"))
B = int(input("Enter the beta value:"))
N = int(input("Enter the order of the matrix:"))
matrix = np.zeros((N,N))

for i in range (N):
    for j in range (N):
        if i == j:
            matrix[i][j] = A
        elif j == i+1 :
            matrix[i][j] = B
        elif j == i-1 :
            matrix[i][j] = B

#printing the matrix
print(matrix)

#finding eigenvalues
w,v = np.linalg.eig(matrix)
print(w)
q = w.sort() #Arranged in ascending order

wid=math.sqrt(N)
div=int(wid)


plt.hist(w,bins= div,color ='r')

d = w[N-1] - w[0]
step = d/N
print(step)
xlegend = plt.xlabel('Eigen value')
ylegend = plt.ylabel('Density of eigen states')

plt.title(f'For dimension N={N}')
plt.show()
```

A. Plots for varying β values(E_o=10, N=1000 are constant)

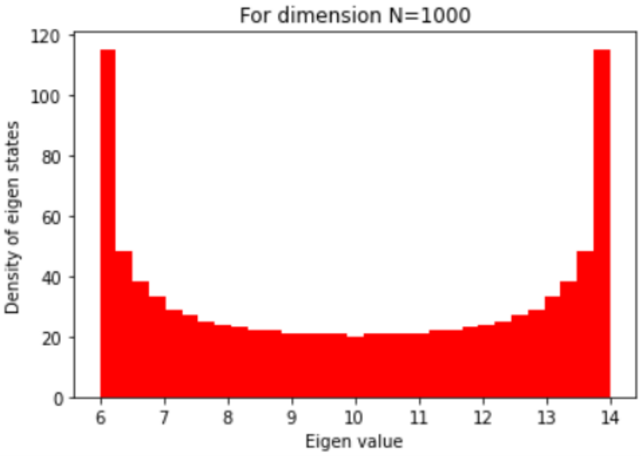

Figure 1: Plot for β=-2

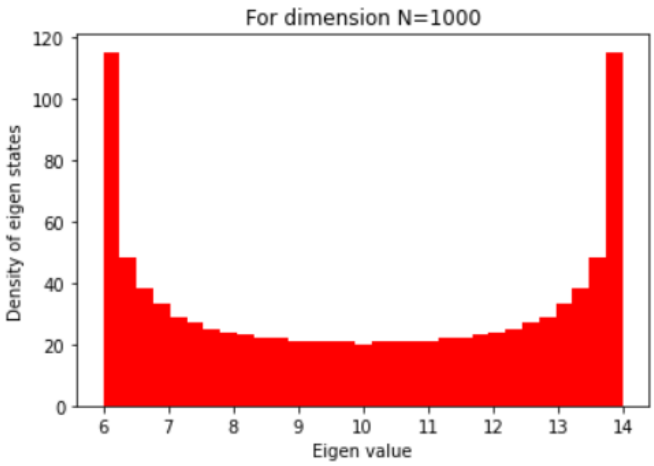

Figure 2: Plot for β=2

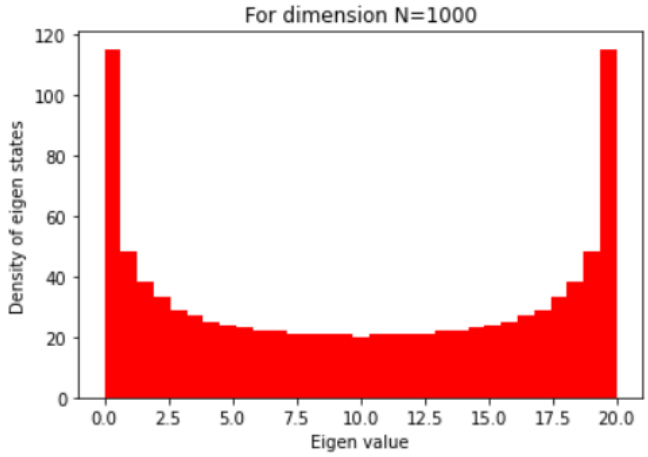

Figure 3: Plot for β=5

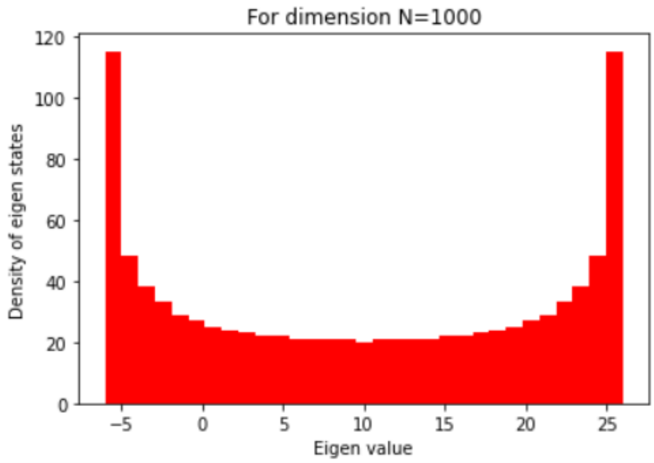

Figure 4: Plot for β=8

B. Plots for increasing N(E_o=10, β=2 are constant)

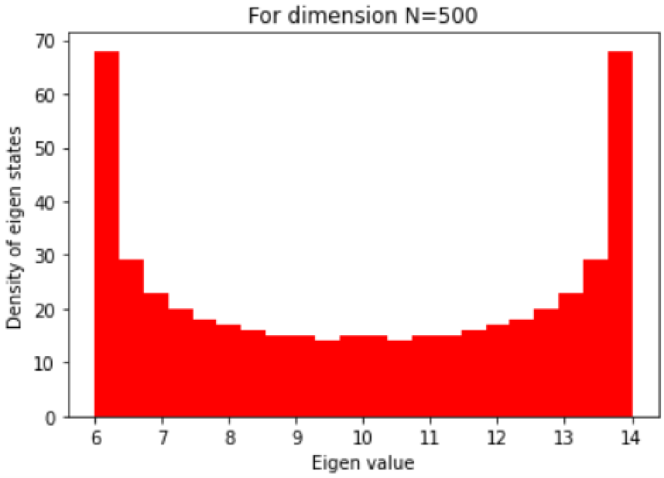

Figure 5: Plot for N=500

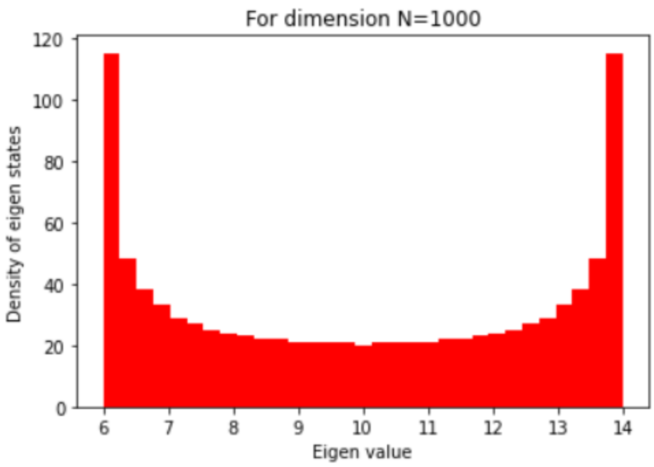

Figure 6: Plot for N=1000

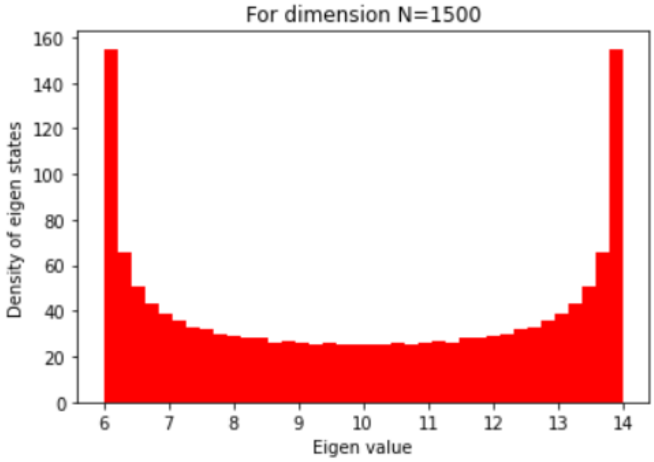

Figure 7: Plot for N=1500

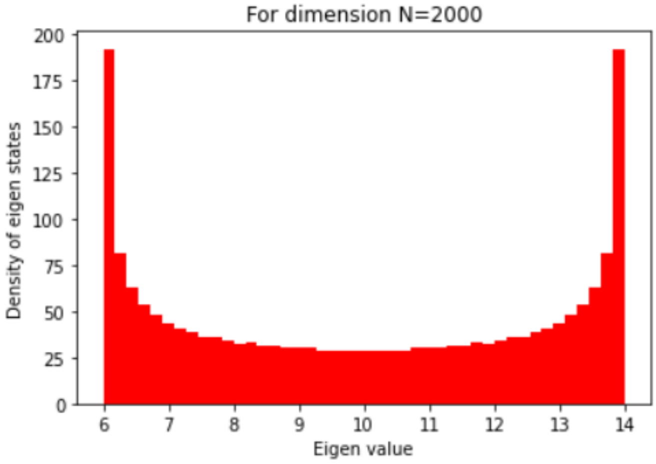

Figure 8: Plot for N=2000

II. DIATOMIC MOLECULES

```
import numpy as np
import matplotlib.pyplot as plt
import math
#Creating the matrix
A1 = int(input("Enter the E1 value:"))
A2 = int(input("Enter the E2 value:"))
B = int(input("Enter the beta value:"))
N = int(input("Enter the order of the matrix:"))

matrix = np.zeros((N,N))
for i in range (N):
    for j in range (N):
        if i == j:
            if i % 2 == 0:
                matrix[i][j] = A2
            else:
                matrix[i][j] = A1
        elif j == i+1 :
            matrix[i][j] = B
        elif j == i-1 :
            matrix[i][j] = B
#printing the matrix
print(matrix)

#finding eigen values
w,v = np.linalg.eig(matrix)
print(w)
q = w.sort() #Arranged in ascending order
plt.hist(w,bins = 90,color ='r')

d = w[N-1] - w[0]
step = d/N
print(step)
xlegend = plt.xlabel('Eigen value')
ylegend = plt.ylabel('Density of eigen states')

plt.title(f'For dimension N={N}')
plt.show()
```

A. Plots for varying β values(E_1=10, E_2=8, N=1000 are constant)

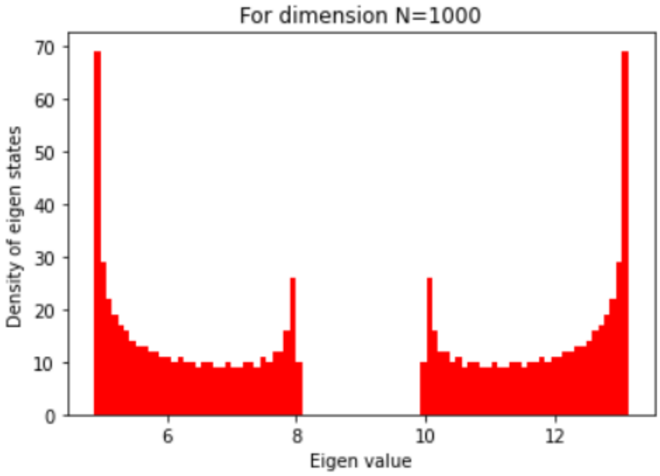

Figure 9: Plot for β=-2

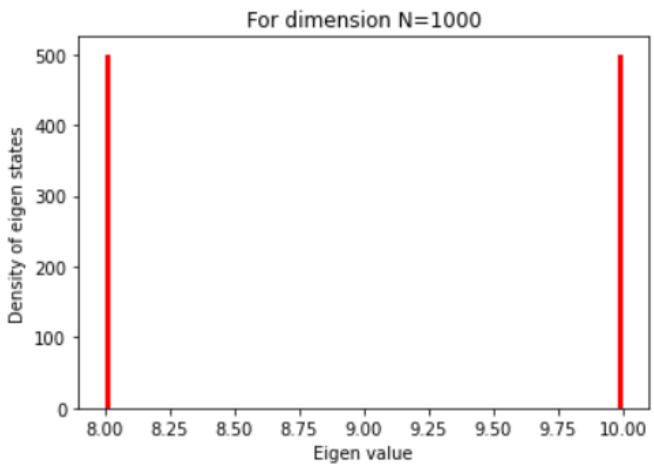

Figure 10: Plot for β=0

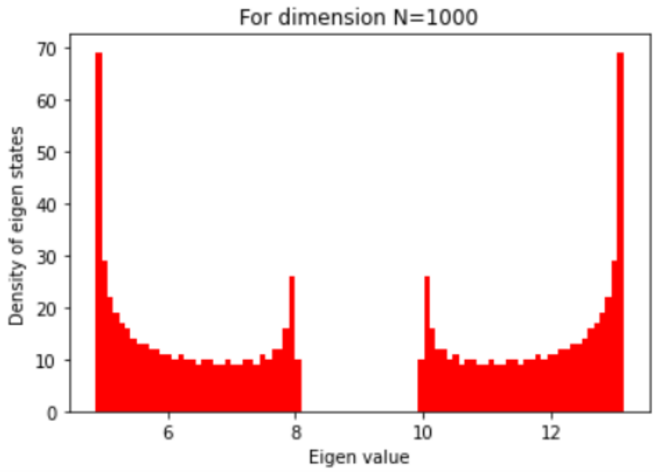

Figure 11: Plot for β=2

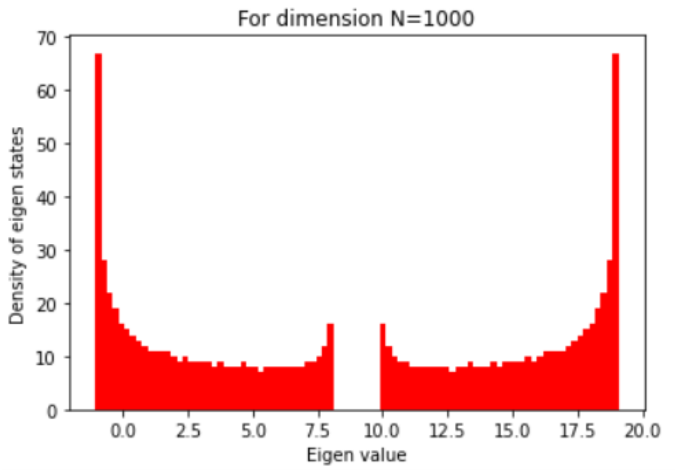

Figure 12: Plot for β=5

B. Plots for increasing N(E_1=10, E_2=8, β=5 are constant)

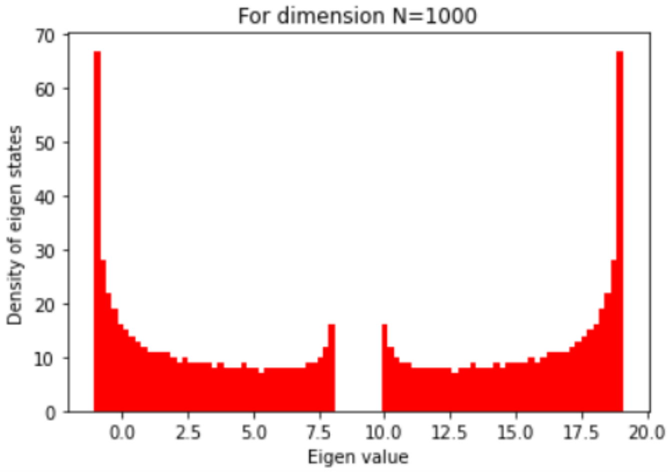

Figure 13: Plot for N=1000

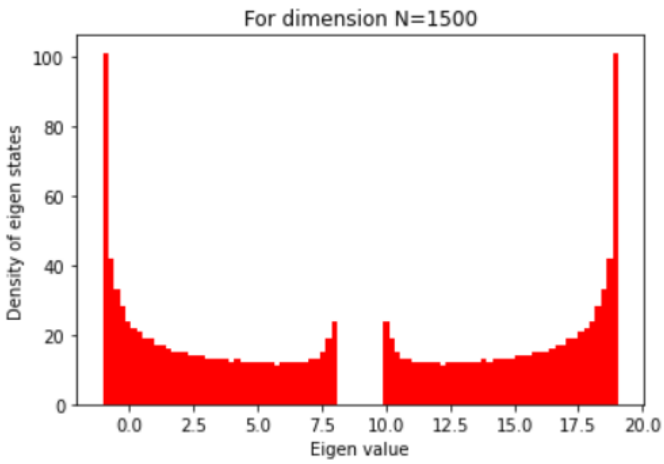

Figure 14: Plot for N=1500

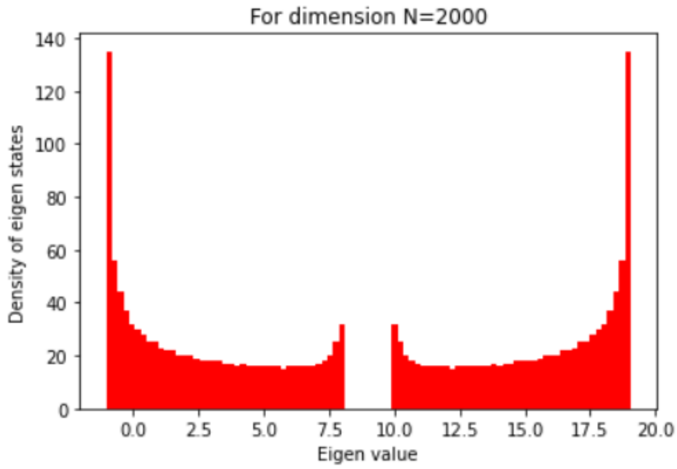

Figure 15: Plot for N=2000

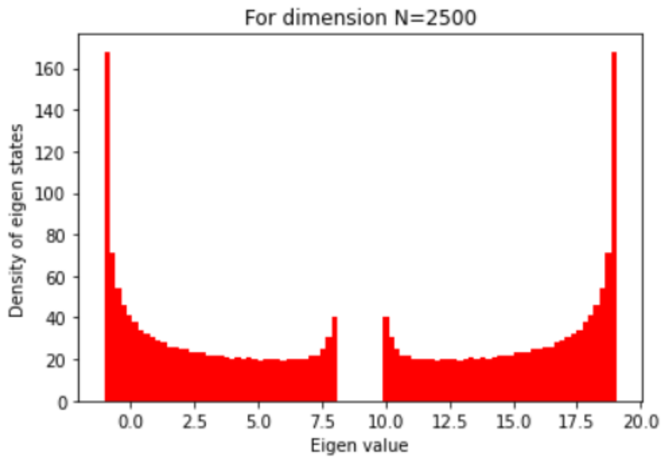

Figure 16: Plot for N=2500

III. MONOATOMIC MOLECULES(RING)

```python
import numpy as np
import matplotlib.pyplot as plt
import math
#Creating the matrix
A = int(input("Enter the diagonal value:"))
B = int(input("Enter the beta value:"))
N = int(input("Enter the order of the matrix:"))
matrix = np.zeros((N,N))
#print the matrix
for i in range (N):
    for j in range (N):
        if i == j:
            matrix[i][j] = A
        elif j == i+1 :
            matrix[i][j] = B
        elif j == i-1 :
            matrix[i][j] = B

for i in range(N):
    for j in range(N):
        if i == N-1 and j==0:
            matrix[i][j] = B
        elif i == 0 and j == N-1:
            matrix[i][j] = B

print(matrix) #Starting matrix is constructed.

#finding eigenvalues
w,v = np.linalg.eig(matrix)
print(w)
q = w.sort() #Arranged in ascending order

wid=math.sqrt(N)
div=int(wid)


plt.hist(w,bins= div,color ='r')

d = w[N-1] - w[0]
step = d/N
print(step)
xlegend = plt.xlabel('Eigen value')
ylegend = plt.ylabel('Density of eigen states')

plt.title(f'For dimension N={N}')
plt.show()
```

A. Plots for varying β values(E_o=10, N=1000 are constant)

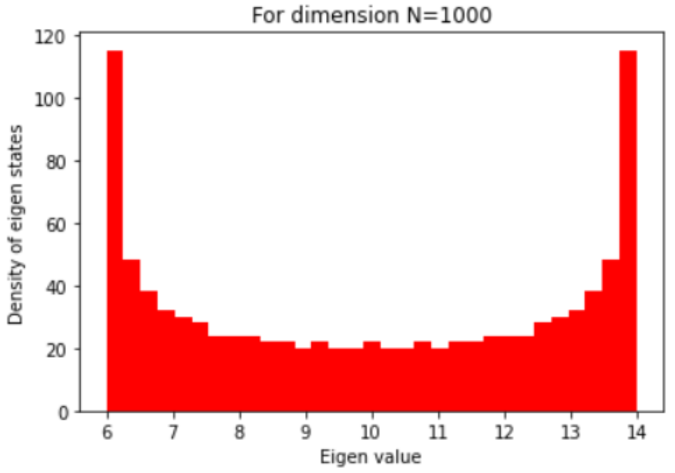

Figure 17: Plot for β=-2

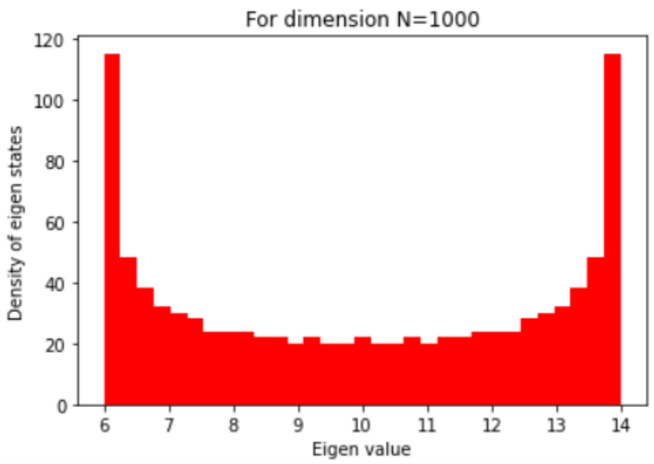

Figure 18: Plot for β=2

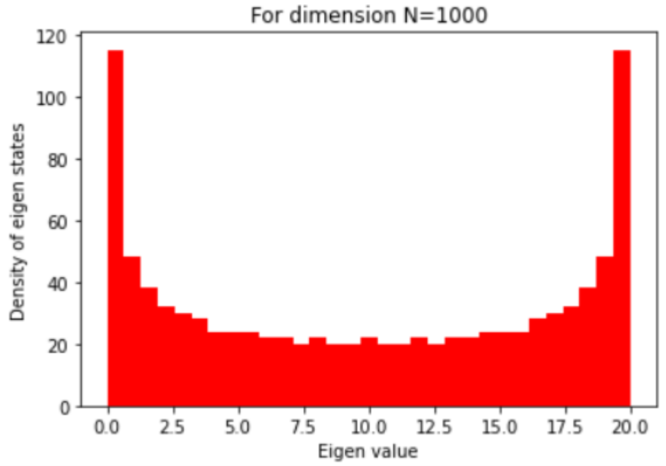

Figure 19: Plot for β=5

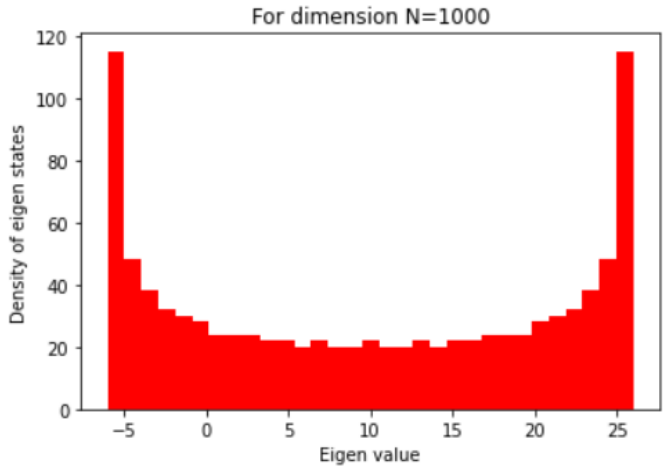

Figure 20: Plot for β=8

B. Plots for increasing N(E_o=10, β=2 are constant)

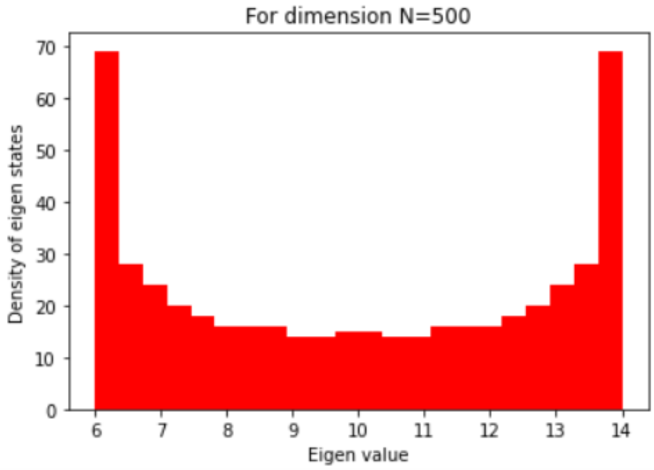

Figure 21: Plot for N=500

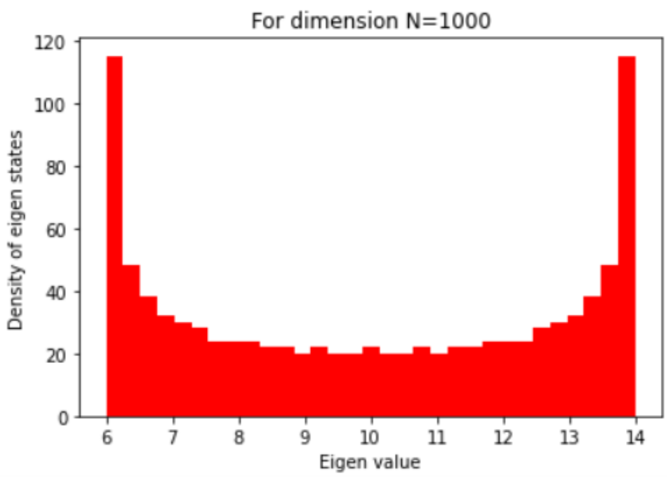

Figure 22: Plot for N=1000

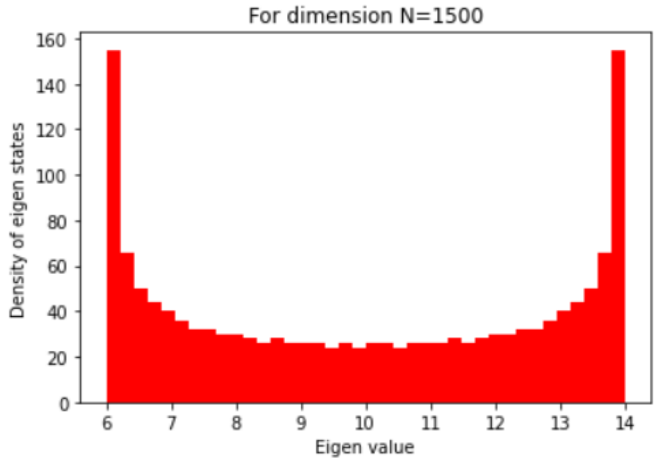

Figure 23: Plot for N=1500

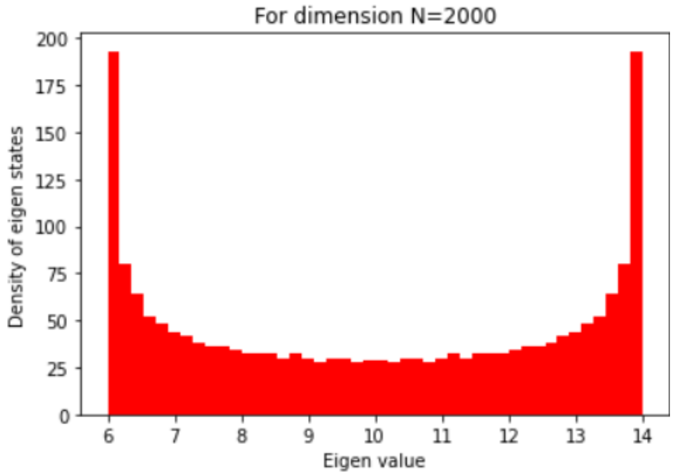

Figure 24: Plot for N=2000

IV. DIATOMIC MOLECULES(RING)

```
import numpy as np
import matplotlib.pyplot as plt
import math
#Creating the matrix
A1 = int(input("Enter the E1 value:"))
A2 = int(input("Enter the E2 value:"))
B = int(input("Enter the beta value:"))
N = int(input("Enter the order of the matrix:"))

matrix = np.zeros((N,N))
for i in range (N):
    for j in range (N):
        if i == j:
            if i % 2 == 0:
                matrix[i][j] = A2
            else:
                matrix[i][j] = A1
        elif j == i+1 :
            matrix[i][j] = B
        elif j == i-1 :
            matrix[i][j] = B

for i in range(N):
    for j in range(N):
        if i == N-1 and j==0:
            matrix[i][j] = B
        elif i == 0 and j == N-1:
            matrix[i][j] = B
#printing the matrix
print(matrix)

#finding eigen values
w,v = np.linalg.eig(matrix)
print(w)
q = w.sort() #Arranged in ascending order
plt.hist(w,bins = 90,color ='r')

d = w[N-1] - w[0]
step = d/N
print(step)
xlegend = plt.xlabel('Eigen value')
ylegend = plt.ylabel('Density of eigen states')

plt.title(f'For dimension N={N}')
plt.show()
```

A. Plots for varying β values(E_1=10, E_2=8, N=1000 are constant)

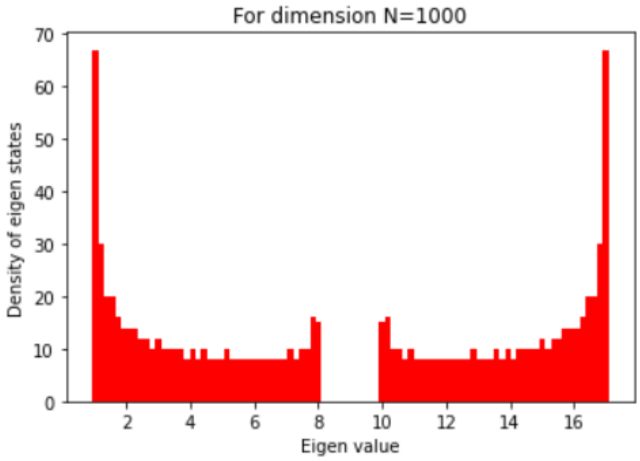

Figure 25: Plot for β=-4

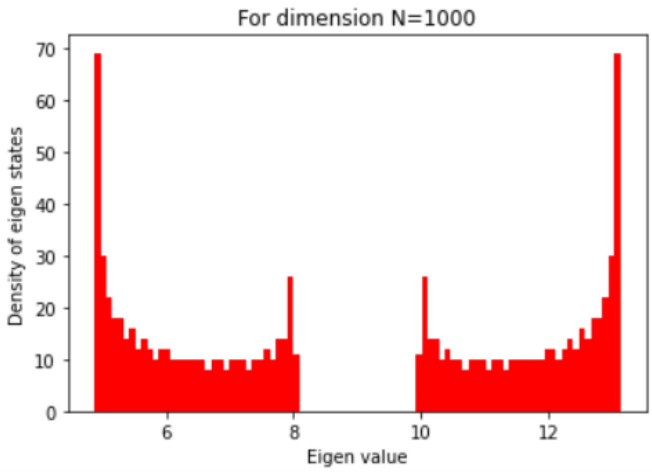

Figure 26: Plot for β=2

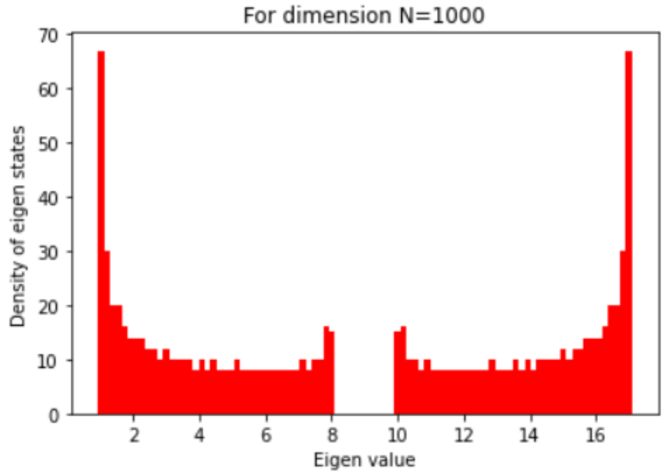

Figure 27: Plot for β=4

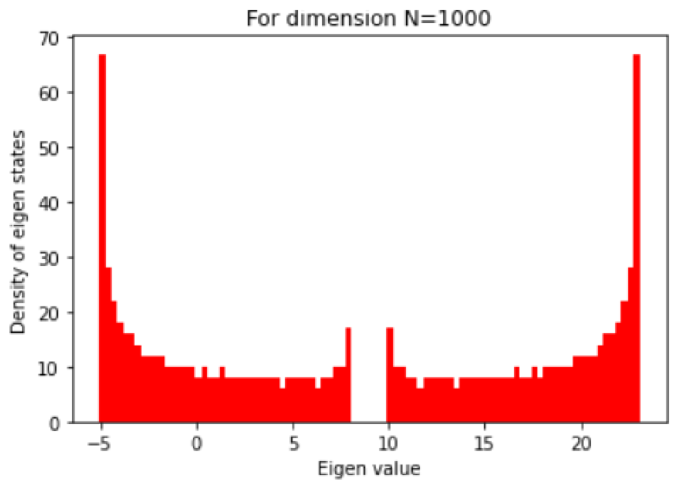

Figure 28: Plot for β=7

B. Plots for increasing N(E_1=10, E_2=8, β=4 are constant)

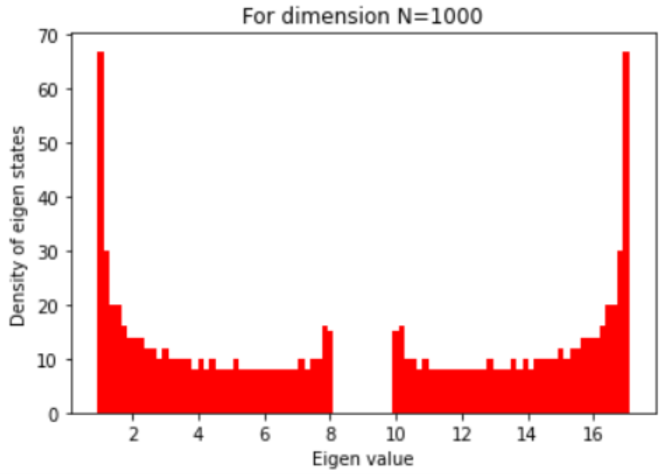

Figure 29: Plot for N=1000

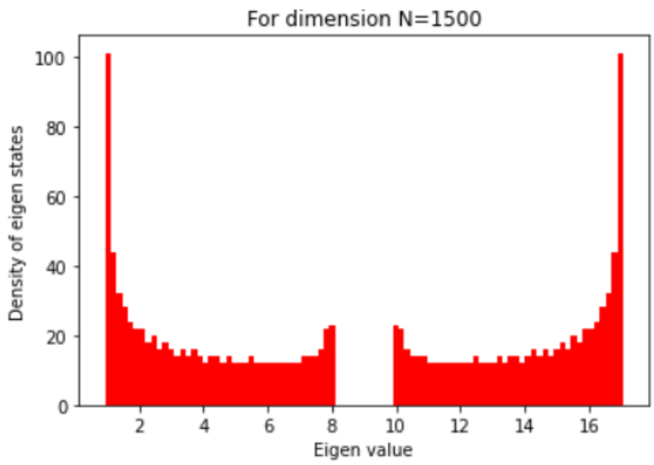

Figure 30: Plot for N=1500

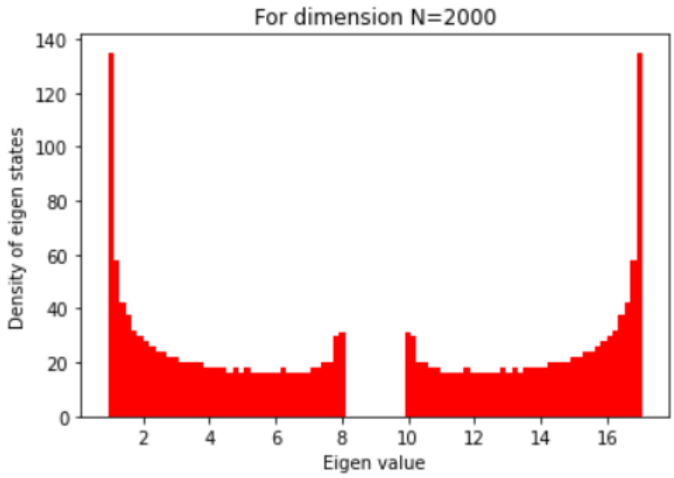

Figure 31: Plot for N=2000

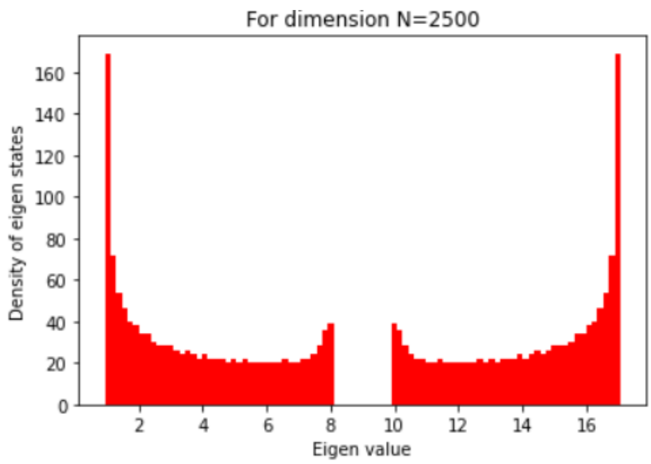

Figure 32: Plot for N=2500

V. OBSERVATIONS

- The plots obtained are dependent on the absolute value of β. A positive or negative sign on β does not affect the values.
- With increasing value of β the eigenvalues for the matrices tend to spread across a broader range.
- The characteristic density of states increases with increasing N in all cases.
- In case of diatomic molecule, the characteristic band gap i s observed in the plot for both the chain and ring structure.