

ASSIGNMENT 1

Physics of Atoms and Molecules

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I. MONOATOMIC MOLECULES

```
1 import numpy as np
2 import matplotlib.pyplot as plt
3 import math
4 #Creating the matrix
5 A = int(input("Enter the diagonal value:"))
6 B = int(input("Enter the beta value:"))
7 N = int(input("Enter the order of the matrix:"))
8 matrix = np.zeros((N,N))
9
10
11 for i in range (N):
12     for j in range (N):
13         if i == j:
14             matrix[i][j] = A
15         elif j == i+1 :
16             matrix[i][j] = B
17         elif j == i-1 :
18             matrix[i][j] = B
19
20 #printing the matrix
21 print(matrix)
22
23 #finding eigenvalues
24 w,v = np.linalg.eig(matrix)
25 print(w)
26 q = w.sort() #Arranged in ascending order
27
28 wid=math.sqrt(N)
29 div=int(wid)
30
31
32 plt.hist(w,bins= div,color = 'r')
33
34 d = w[N-1] - w[0]
35 step = d/N
36 print(step)
37 xlegend = plt.xlabel('Eigen value')
38 ylegend = plt.ylabel('Density of eigen states')
39
40 plt.title(f'For dimension N={N}')
41 plt.show()
```

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

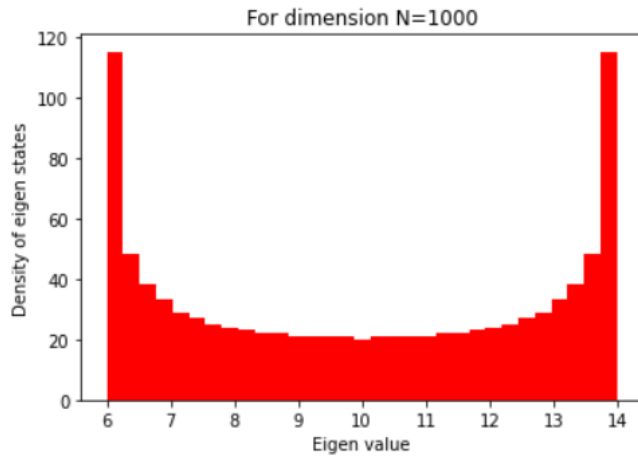


Figure 1: Plot for $\beta=-2$

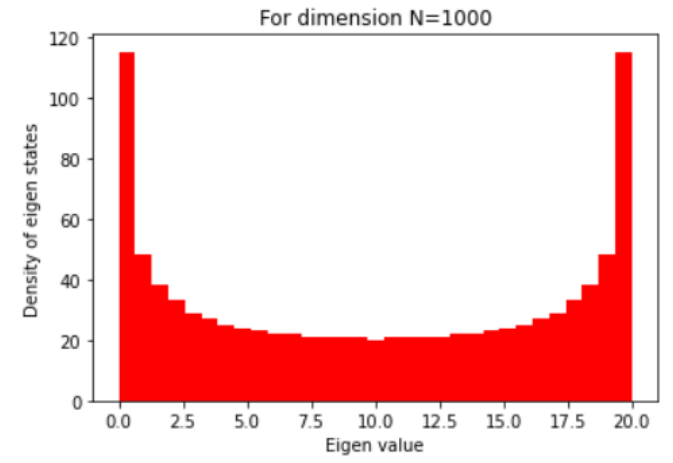


Figure 3: Plot for $\beta=5$

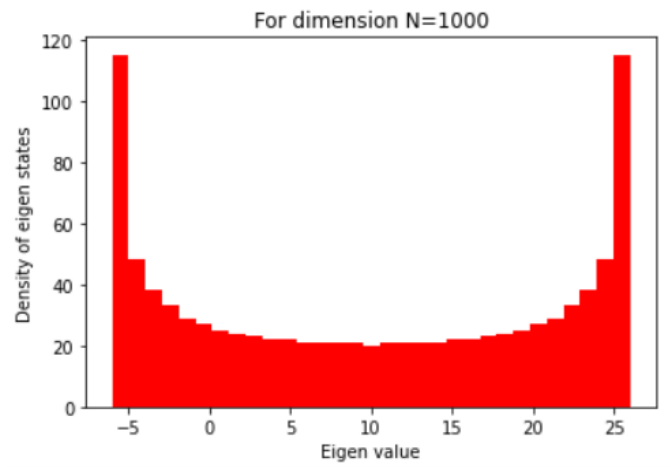


Figure 4: Plot for $\beta=8$

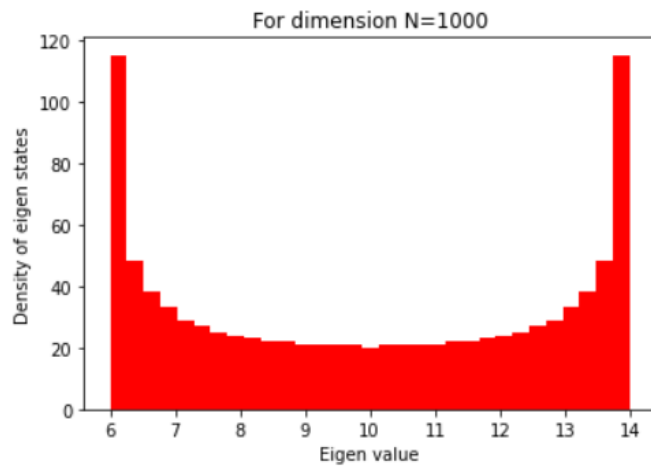


Figure 2: Plot for $\beta=2$

B. Plots for increasing N ($E_o=10$, $\beta=2$ are constant)

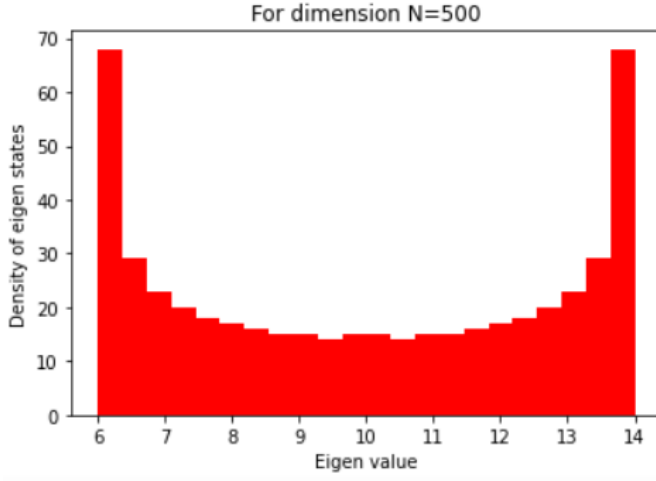


Figure 5: Plot for $N=500$

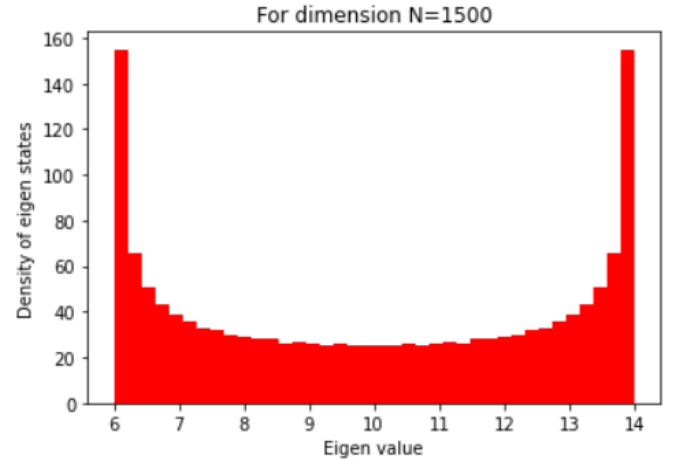


Figure 7: Plot for $N=1500$

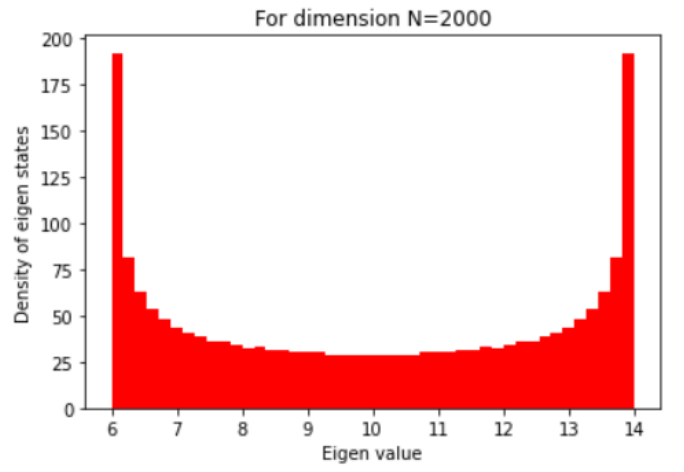


Figure 8: Plot for $N=2000$

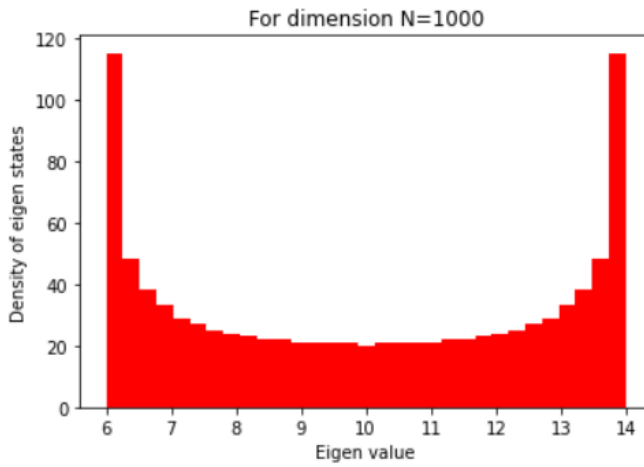


Figure 6: Plot for $N=1000$

II. DIATOMIC MOLECULES

```

1 import numpy as np
2 import matplotlib.pyplot as plt
3 import math
4 #Creating the matrix
5 A1 = int(input("Enter the E1 value:"))
6 A2 = int(input("Enter the E2 value:"))
7 B = int(input("Enter the beta value:"))
8 N = int(input("Enter the order of the matrix:"))
9
10 matrix = np.zeros((N,N))
11 for i in range (N):
12     for j in range (N):
13         if i == j:
14             if i % 2 == 0:
15                 matrix[i][j] = A2
16             else:
17                 matrix[i][j] = A1
18         elif j == i+1 :
19             matrix[i][j] = B
20         elif j == i-1 :
21             matrix[i][j] = B
22 #printing the matrix
23 print(matrix)
24
25 #finding eigen values
26 w,v = np.linalg.eig(matrix)
27 print(w)
28 q = w.sort() #Arranged in ascending order
29 plt.hist(w,bins = 90,color = 'r')
30
31 d = w[N-1] - w[0]
32 step = d/N
33 print(step)
34 xlegend = plt.xlabel('Eigen value')
35 ylegend = plt.ylabel('Density of eigen states')
36
37 plt.title(f'For dimension N={N}')
38 plt.show()

```

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

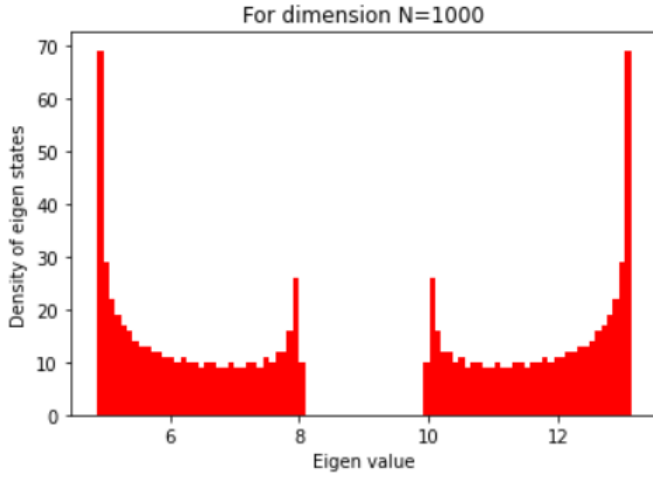


Figure 9: Plot for $\beta=-2$

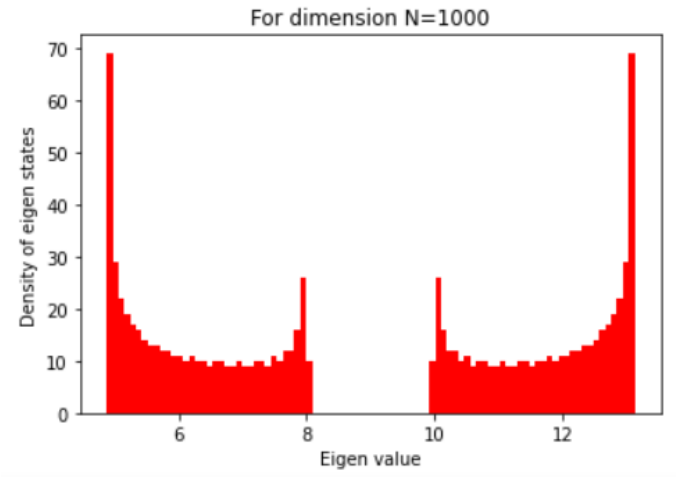


Figure 11: Plot for $\beta=2$

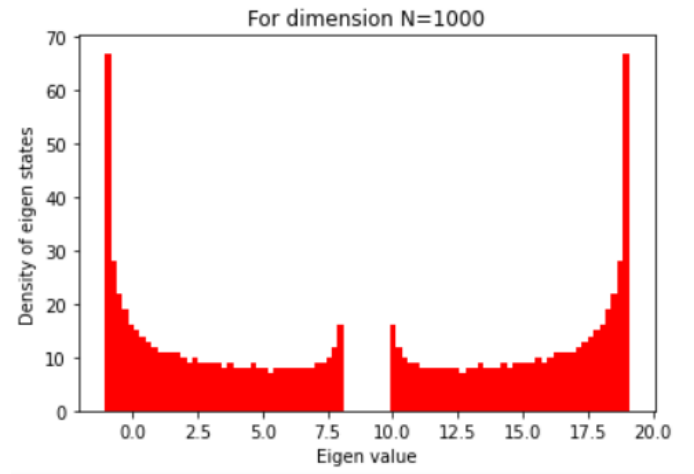


Figure 12: Plot for $\beta=5$

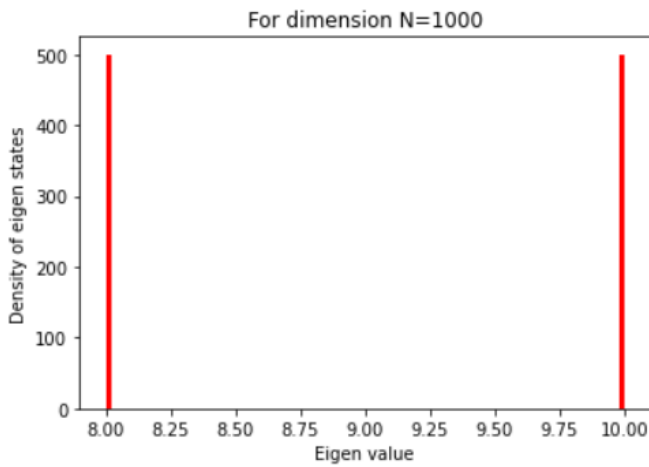


Figure 10: Plot for $\beta=0$

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

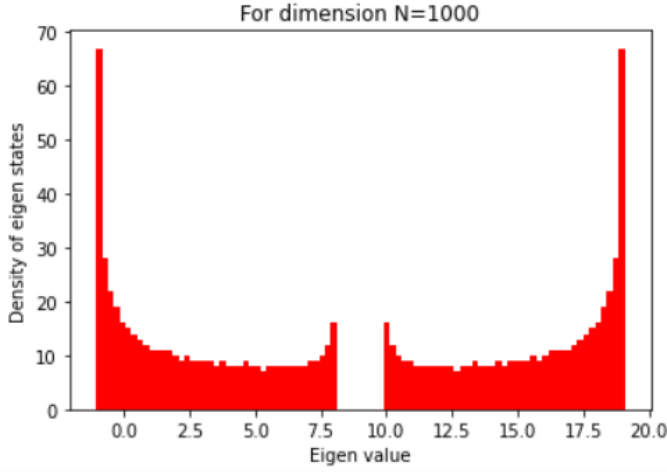


Figure 13: Plot for N=1000

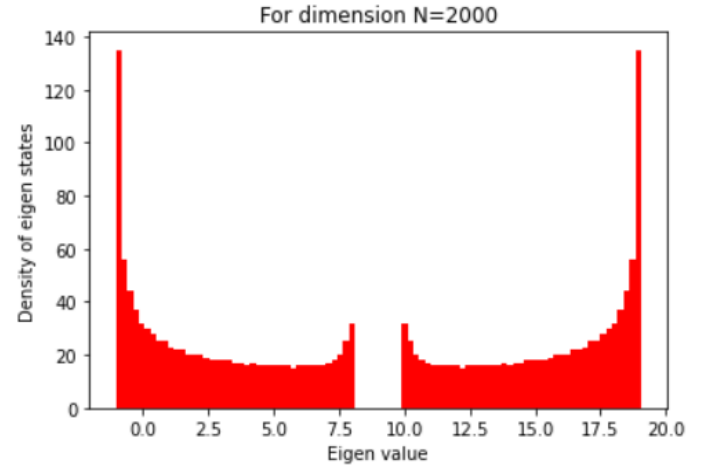


Figure 15: Plot for N=2000

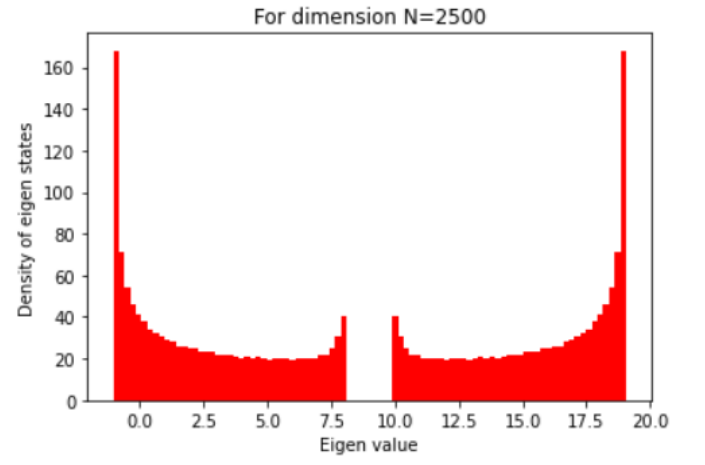


Figure 16: Plot for N=2500

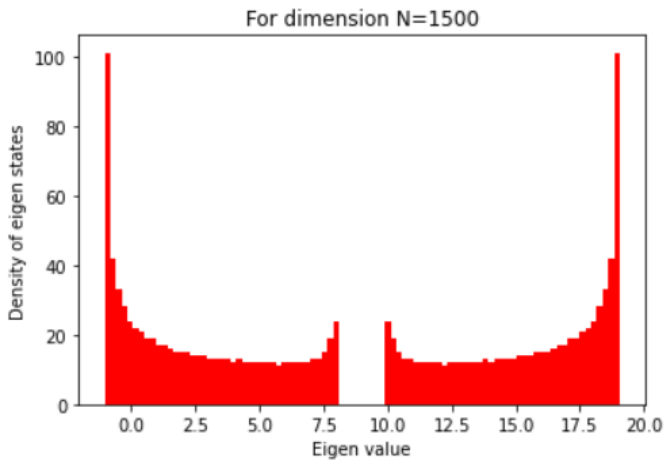


Figure 14: Plot for N=1500

III. MONOATOMIC MOLECULES(RING)

```

1 import numpy as np
2 import matplotlib.pyplot as plt
3 import math
4 #Creating the matrix
5 A = int(input("Enter the diagonal value:"))
6 B = int(input("Enter the beta value:"))
7 N = int(input("Enter the order of the matrix:"))
8 matrix = np.zeros((N,N))
9 #print the matrix
10 for i in range (N):
11     for j in range (N):
12         if i == j:
13             matrix[i][j] = A
14         elif j == i+1 :
15             matrix[i][j] = B
16         elif j == i-1 :
17             matrix[i][j] = B
18
19 for i in range(N):
20     for j in range(N):
21         if i == N-1 and j==0:
22             matrix[i][j] = B
23         elif i == 0 and j == N-1:
24             matrix[i][j] = B
25
26 print(matrix) #Starting matrix is constructed.
27
28 #finding eigenvalues
29 w,v = np.linalg.eig(matrix)
30 print(w)
31 q = w.sort() #Arranged in ascending order
32
33 wid=math.sqrt(N)
34 div=int(wid)
35
36
37 plt.hist(w,bins= div,color = 'r')
38
39 d = w[N-1] - w[0]
40 step = d/N
41 print(step)
42 xlegend = plt.xlabel('Eigen value')
43 ylegend = plt.ylabel('Density of eigen states')
44
45 plt.title(f'For dimension N={N}')
46 plt.show()

```

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

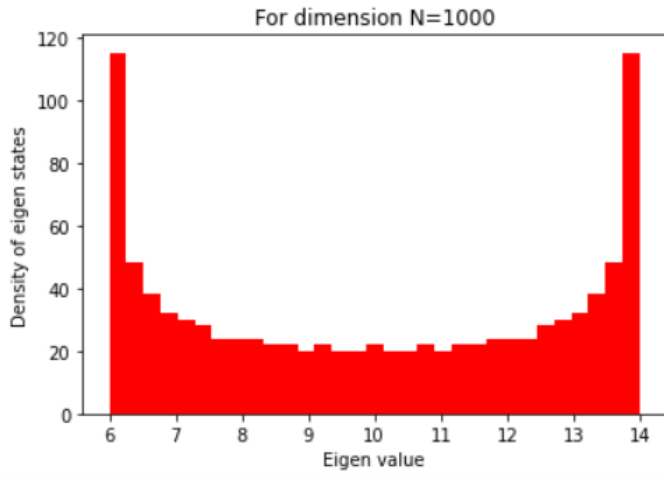


Figure 17: Plot for $\beta=-2$

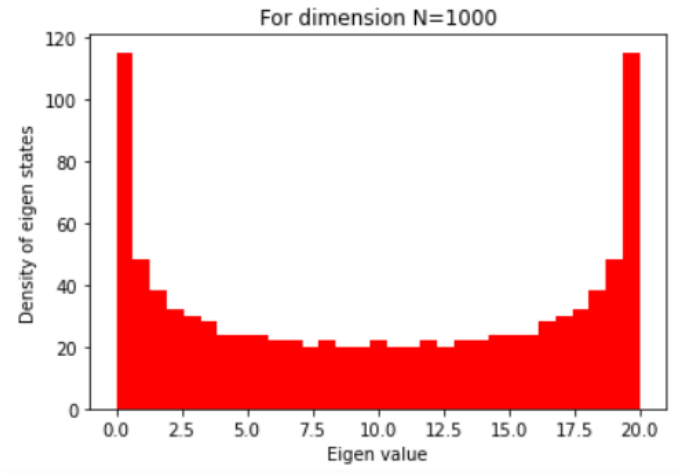


Figure 19: Plot for $\beta=5$

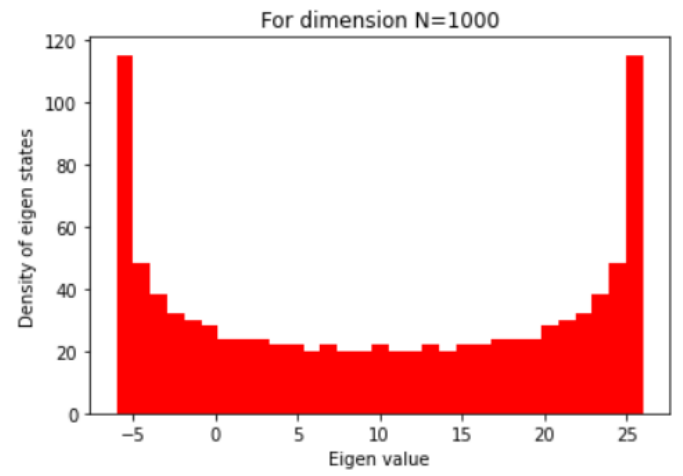


Figure 20: Plot for $\beta=8$

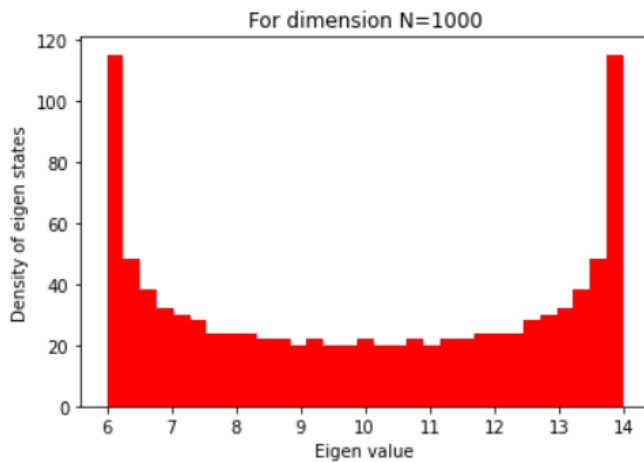


Figure 18: Plot for $\beta=2$

B. Plots for increasing N ($E_o=10$, $\beta=2$ are constant)

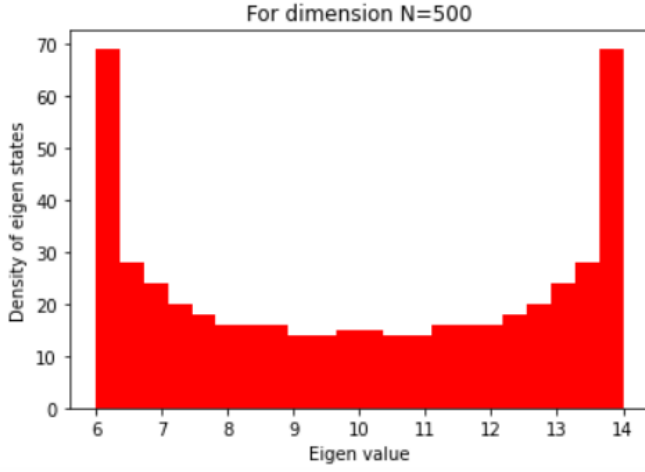


Figure 21: Plot for $N=500$

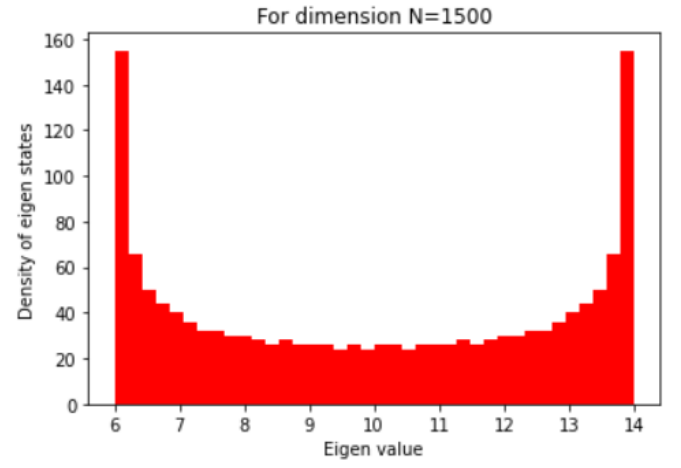


Figure 23: Plot for $N=1500$

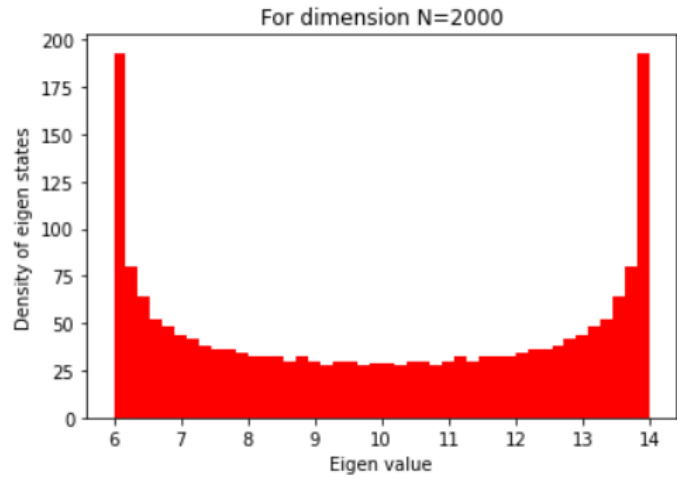


Figure 24: Plot for $N=2000$

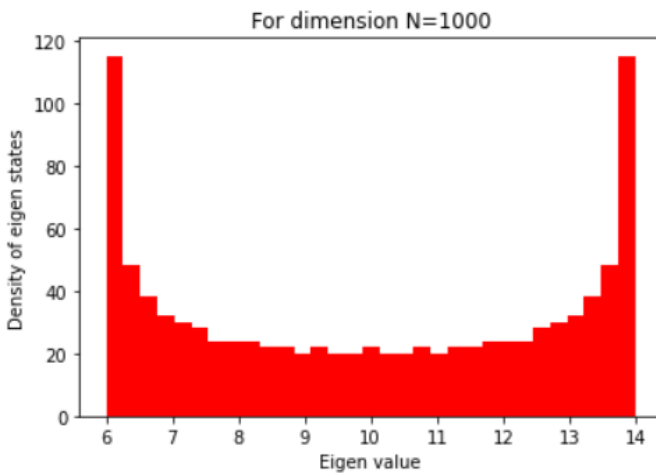


Figure 22: Plot for $N=1000$

IV. DIATOMIC MOLECULES(RING)

```

1 import numpy as np
2 import matplotlib.pyplot as plt
3 import math
4 #Creating the matrix
5 A1 = int(input("Enter the E1 value:"))
6 A2 = int(input("Enter the E2 value:"))
7 B = int(input("Enter the beta value:"))
8 N = int(input("Enter the order of the matrix:"))
9
10 matrix = np.zeros((N,N))
11 for i in range (N):
12     for j in range (N):
13         if i == j:
14             if i % 2 == 0:
15                 matrix[i][j] = A2
16             else:
17                 matrix[i][j] = A1
18         elif j == i+1 :
19             matrix[i][j] = B
20         elif j == i-1 :
21             matrix[i][j] = B
22
23 for i in range(N):
24     for j in range(N):
25         if i == N-1 and j==0:
26             matrix[i][j] = B
27         elif i == 0 and j == N-1:
28             matrix[i][j] = B
29 #printing the matrix
30 print(matrix)
31
32 #finding eigen values
33 w,v = np.linalg.eig(matrix)
34 print(w)
35 q = w.sort() #Arranged in ascending order
36 plt.hist(w,bins = 90,color = 'r')
37
38 d = w[N-1] - w[0]
39 step = d/N
40 print(step)
41 xlegend = plt.xlabel('Eigen value')
42 ylegend = plt.ylabel('Density of eigen states')
43
44 plt.title(f'For dimension N={N}')
45 plt.show()

```

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

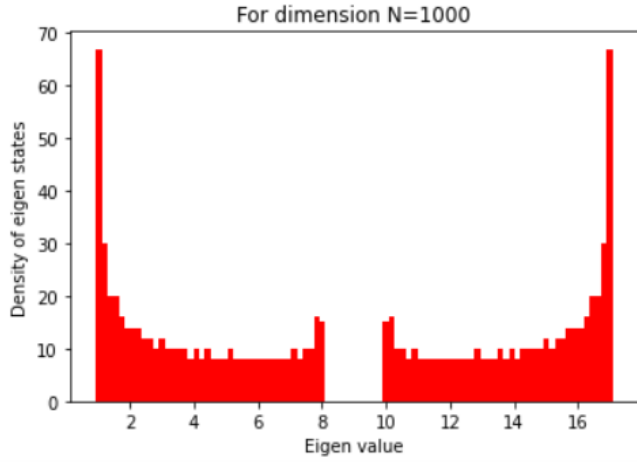


Figure 25: Plot for $\beta=-4$

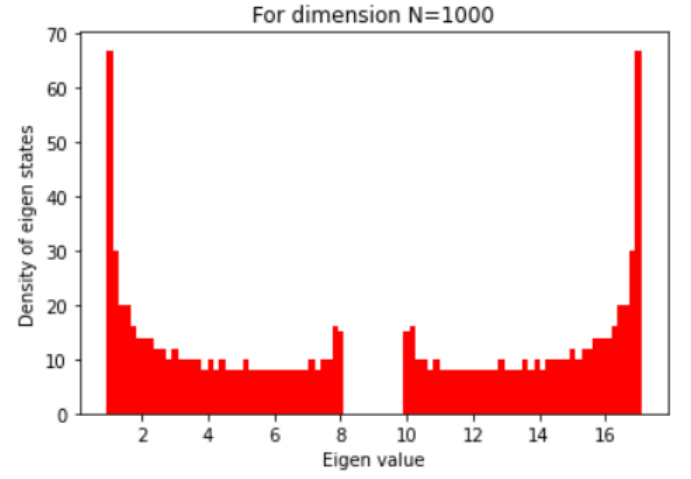


Figure 27: Plot for $\beta=4$

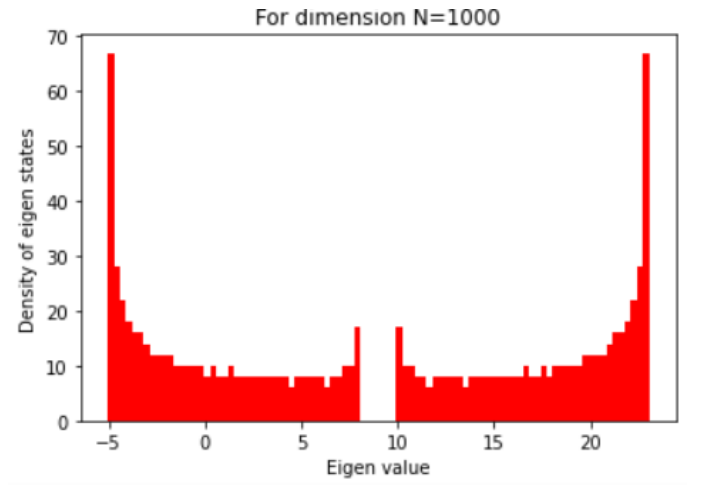


Figure 28: Plot for $\beta=7$

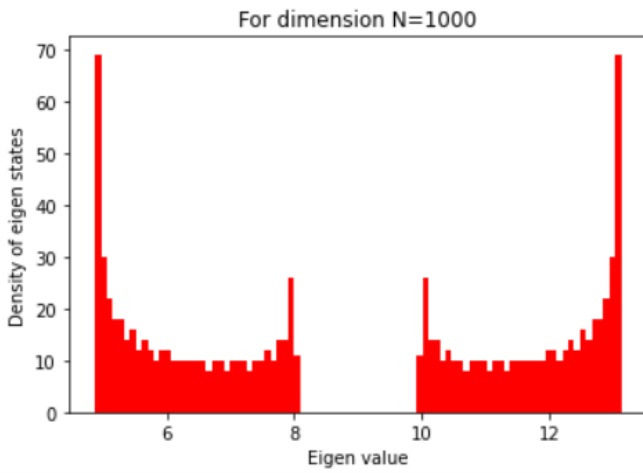


Figure 26: Plot for $\beta=2$

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

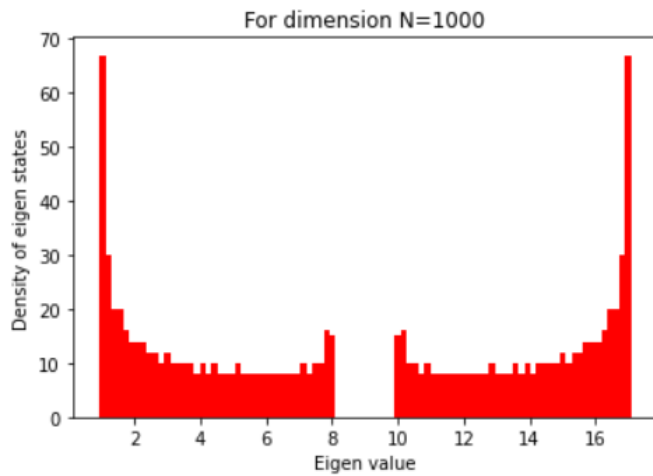


Figure 29: Plot for $N=1000$

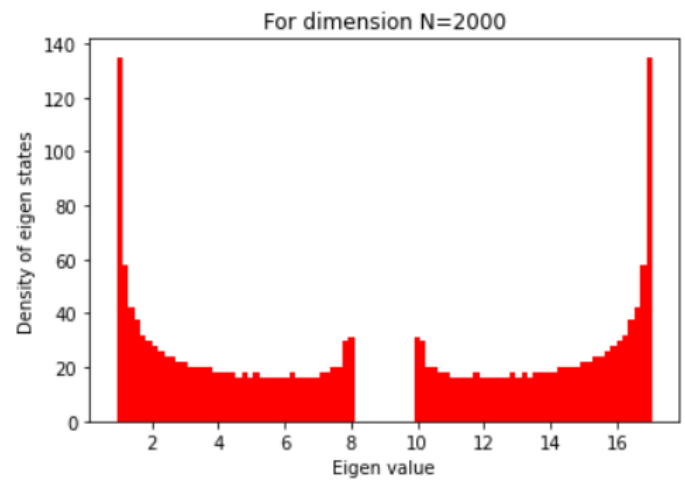


Figure 31: Plot for $N=2000$

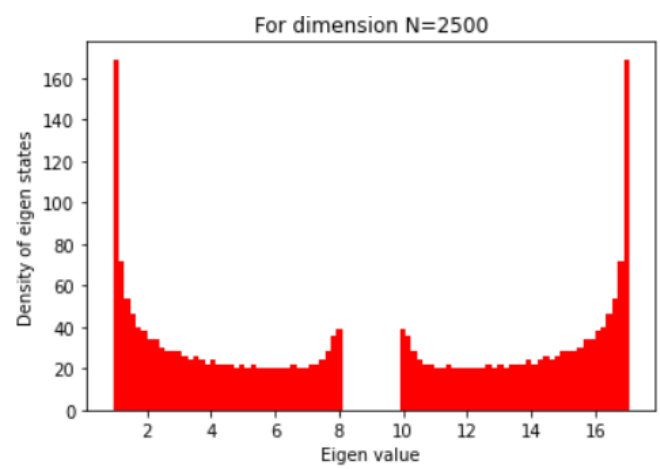


Figure 32: Plot for $N=2500$

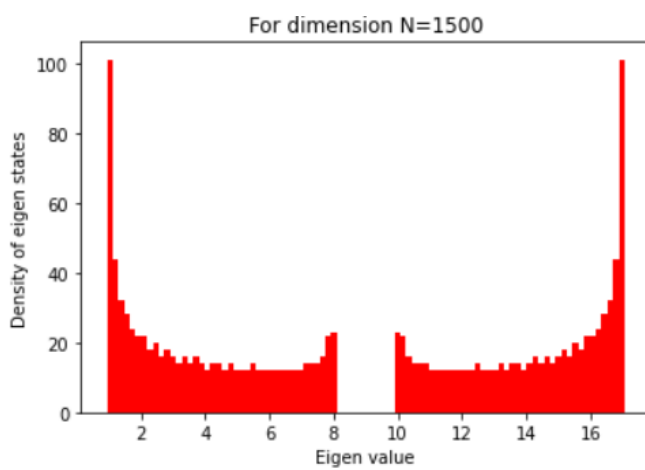


Figure 30: Plot for $N=1500$

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 is observed in the plot for both the chain and ring structure.