3-D Hydrogen Atom

January 11, 2018

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In [14]: import numpy as np
         import matplotlib.pyplot as pt
         import numpy.linalg as la
         import scipy.sparse.linalg as lin
         from mpl_toolkits.mplot3d import Axes3D
         from scipy.interpolate import griddata
         import seaborn as sns
         %matplotlib inline
         # %matplotlib qt
```

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In [27]: # When numerically solving the structure of hydrogen atom using finite difference metho
         # the main objective is to establish 1-1 correspondence between the col vector which re
         # (000) (001)....(NNN), with the horizontal location of matrix (0,1...N^3) to put value
         # matrix where the numbers should be calculated.
         # if we focus on certain point (x,y,z), it has a location in the col vector, and its ne
         # has various positions in the horizontal row in the matrix, and we need to find the po
         # build the identification-table.

         L = 31 # dimension of the box
         N = 20 # Accuracy; even number
         location = []
         for i in range(0,N):
             for j in range(0,N):
                 for k in range(0,N):
                     location.append((i,j,k)) # (000),001,...00N, 011,...0N1,...0NN, 100, 101...

         def matrix_to_index(a,b,c):
             return location.index((a,b,c)) # e.g (0,0,3)-> 3
         def index_to_ijk(i):
             return location[i] #e.g 5->(0,0,5)

         X = np.linspace(-L/2,L/2,N)
         Y = np.linspace(-L/2,L/2,N)
         Z = np.linspace(-L/2,L/2,N)
         d = X[1]-X[0]

         # Constructing Hamiltonian: -p^2/2m + V(1/r)
         H=np.zeros((N**3,N**3))

         for i in range(0,N**3): # loop all xyz combination
             x = index_to_ijk(i)[0]
             y = index_to_ijk(i)[1]
             z = index_to_ijk(i)[2]

             H[i,matrix_to_index(x,y,z)] = -6   # f''(x) = f''(x+d)-2f(x)+f''(x-d) / d^2 and sum
             if x+1<N:
                 H[i,matrix_to_index(x+1,y,z)] = 1
             if x-1>=0:
                 H[i,matrix_to_index(x-1,y,z)] = 1
             if y+1<N:
                 H[i,matrix_to_index(x,y+1,z)] = 1
             if y-1>=0:
                 H[i,matrix_to_index(x,y-1,z)] = 1
             if z+1<N:
                 H[i,matrix_to_index(x,y,z+1)] = 1
             if z-1>=0:
                 H[i,matrix_to_index(x,y,z-1)] = 1
         H = -H/d**2

         for i in range(0,N**3):
             x = index_to_ijk(i)[0]
             y = index_to_ijk(i)[1]
             z = index_to_ijk(i)[2]
             H[i,i] += -2/np.sqrt(X[x]**2+Y[y]**2+Z[z]**2)
```

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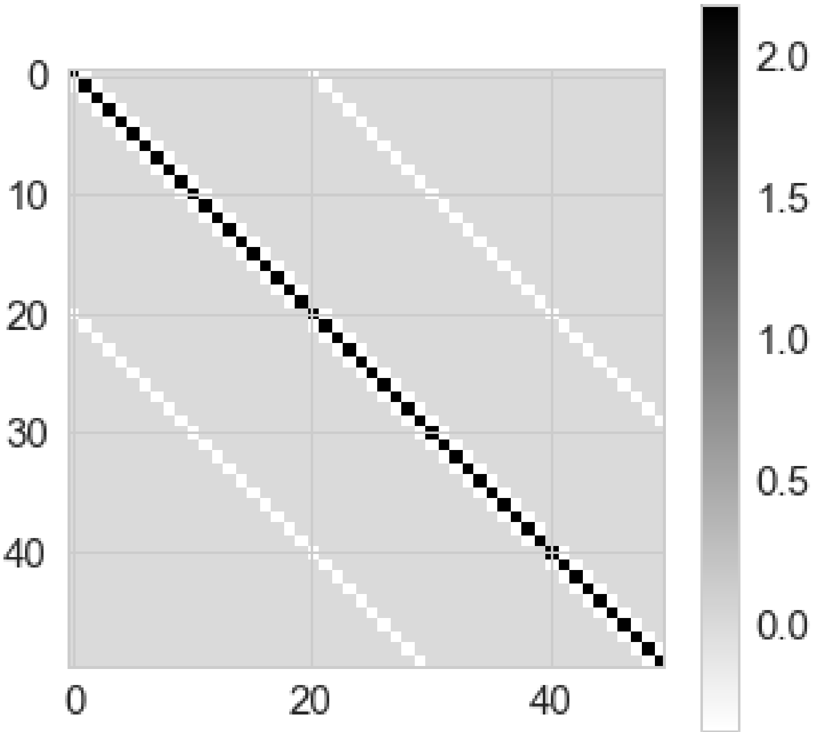
In [28]: sns.set(font_scale=1.5)
         sns.set_style("whitegrid")
         pt.figure(figsize=(5,5))
         pt.imshow(H[0:50,0:50],cmap='gray_r',interpolation='none')
         pt.colorbar()
         pt.show()
```



```
In [29]: # Solving for eigensystem using spars matrix technique

         vals, vecs = lin.eigsh(H,k=20,which='SA') # first k states with lowest energies

In [30]: ## Different energy states
         sns.set(font_scale=1.5)
         sns.set_style("whitegrid")

         for n in range(0,20):     # including ground states
             fig = pt.figure(figsize=(15,6))

             # Density distribution across xy plane

             ax = fig.add_subplot(121, projection='3d')
             ax.tick_params(axis='x', pad=1)
             ax.tick_params(axis='y', pad=1)
             ax.tick_params(axis='z', pad=1)
             xs=[]
             ys=[]
             rho=[]
             for i in range(0,len(vecs[:,0])):
                 if index_to_ijk(i)[2]==0:
                     xs.append(X[index_to_ijk(i)[0]])
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        ys.append(Y[index_to_ijk(i)[1]])
        rho.append(vecs[:,n][i]**2*10**5) # *1000 to make things look nicer

# interpolate
xi = yi = np.arange(-L/2,L/2,1)
xi,yi = np.meshgrid(xi,yi)
zi = griddata((xs,ys),rho,(xi,yi),method='cubic')
pt.contourf(xi,yi,zi,np.arange(0,np.max(rho),np.max(rho)/200),cmap='rainbow',alpha=

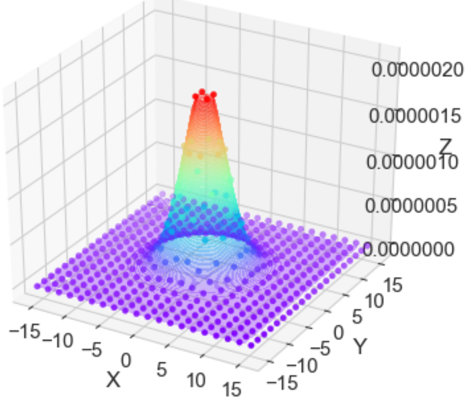
ax.scatter(xs, ys, rho, c=rho, marker='o',cmap='rainbow')
ax.set_xlabel('X')
ax.set_ylabel('Y')
ax.set_zlabel('Z')
pt.title('Density Distrbution across a flat surface')

# Spacial density distribution

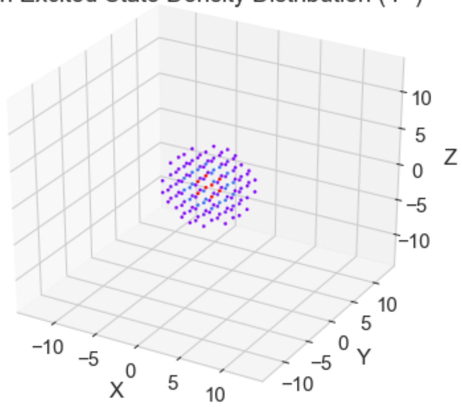
ax = fig.add_subplot(122, projection='3d')
ax.tick_params(axis='x', pad=1)
ax.tick_params(axis='y', pad=1)
ax.tick_params(axis='z', pad=1)
xs=[]
ys=[]
zs=[]
rho=[]
for i in range(0,len(vecs[:,0])):
    xs = np.append(xs, X[index_to_ijk(i)[0]])
    ys = np.append(ys, Y[index_to_ijk(i)[1]])
    zs = np.append(zs, Z[index_to_ijk(i)[2]])
    rho = np.append(rho, vecs[:,n][i]**2)
rho=np.ma.masked_where(rho < 0.0003, rho)

ax.scatter(xs, ys, zs, c=rho, marker='.',alpha=1,cmap='rainbow')
ax.set_xlim(-14,14)
ax.set_ylim(-14,14)
ax.set_zlim(-14,14)
ax.set_xlabel('X')
ax.set_ylabel('Y')
ax.set_zlabel('Z')
pt.title(str(n)+'th Excited State Density Distribution ($\Psi^2$)')
pt.show()
```

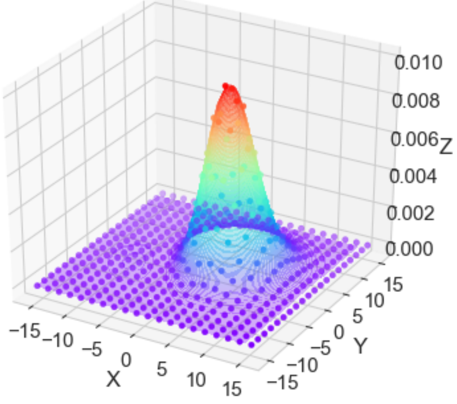
Density Distrbution across a flat surface



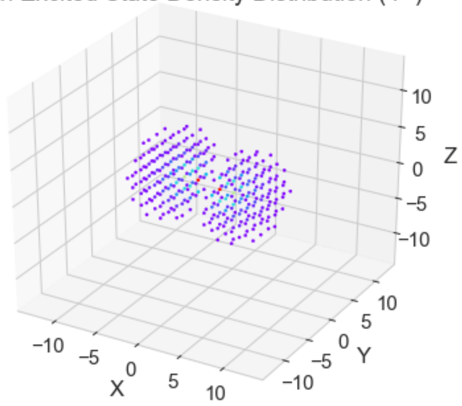
0th Excited State Density Distribution (Ψ^2)



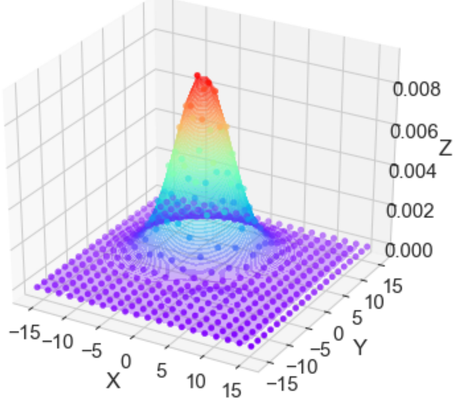
Density Distrbution across a flat surface



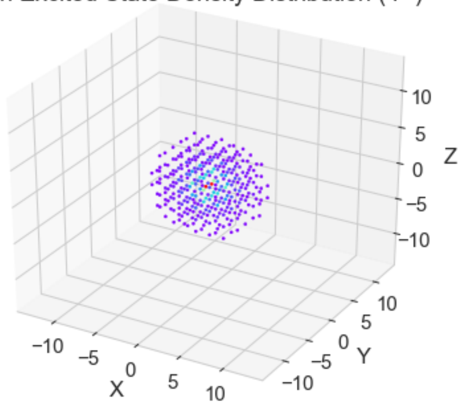
1th Excited State Density Distribution (Ψ^2)



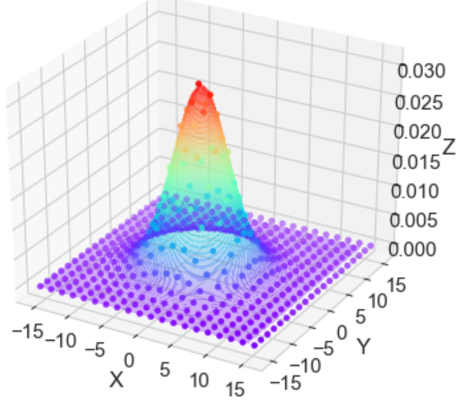
Density Distrbution across a flat surface



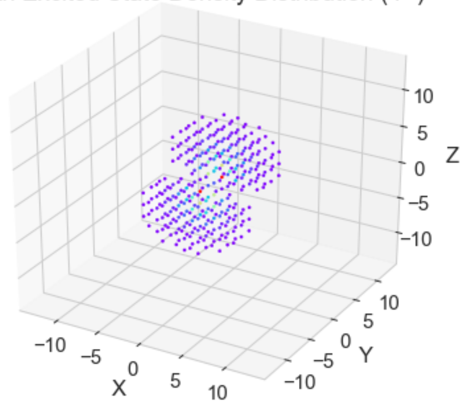
2th Excited State Density Distribution (Ψ^2)



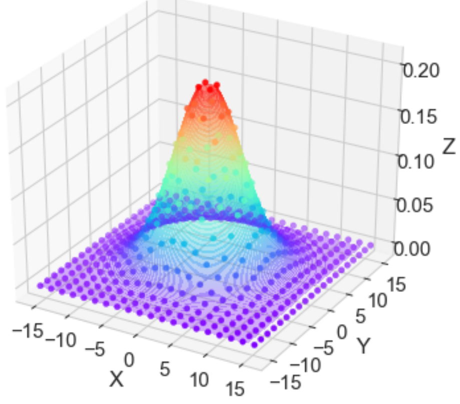
Density Distrbution across a flat surface



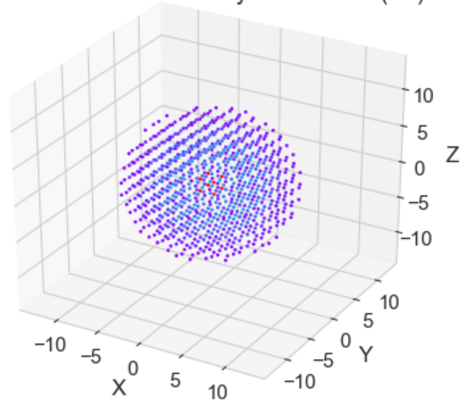
3th Excited State Density Distribution (Ψ^2)



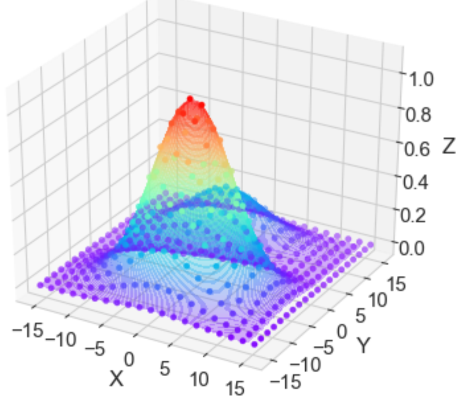
Density Distrbution across a flat surface



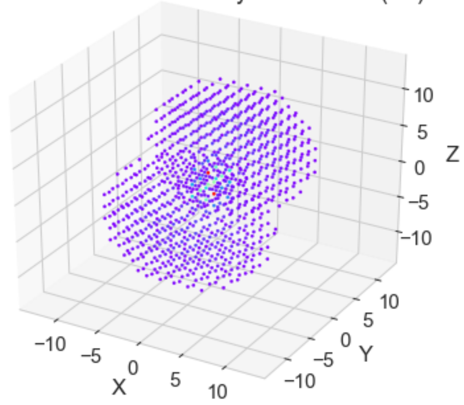
4th Excited State Density Distribution (Ψ^2)

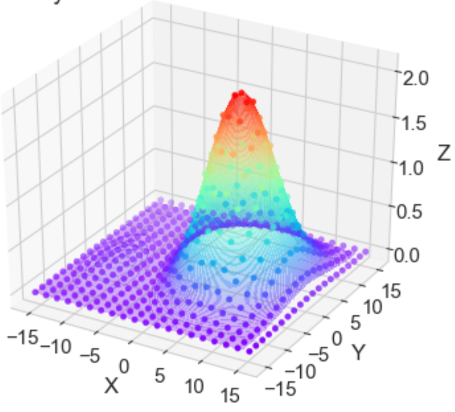


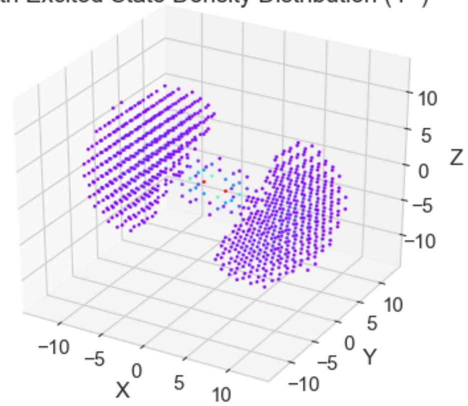
Density Distrbution across a flat surface



5th Excited State Density Distribution (Ψ^2)




Density Distrbution across a flat surface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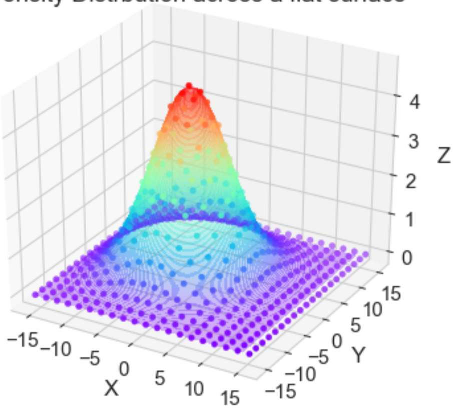
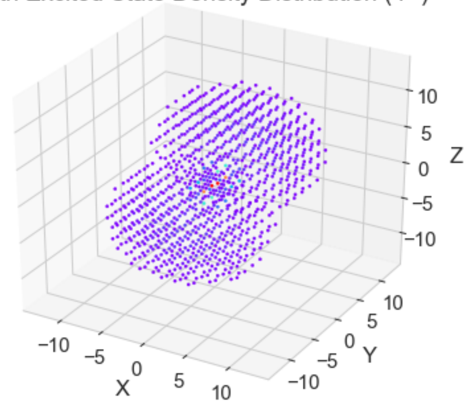

Density Distrbution across a flat surface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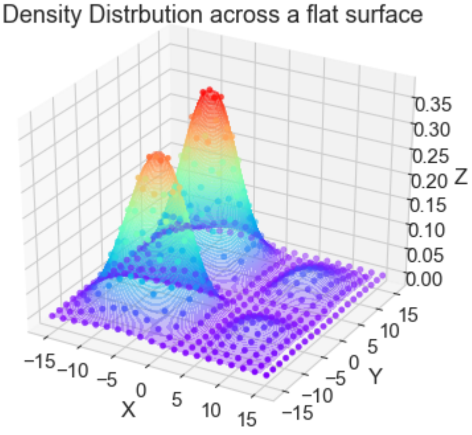
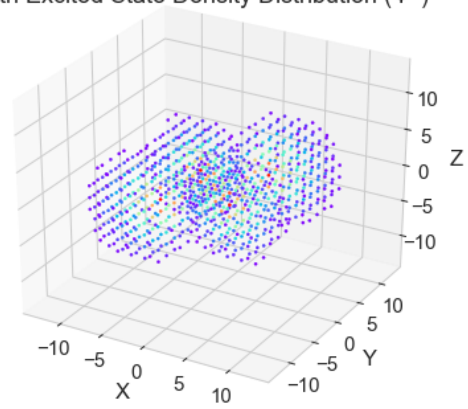
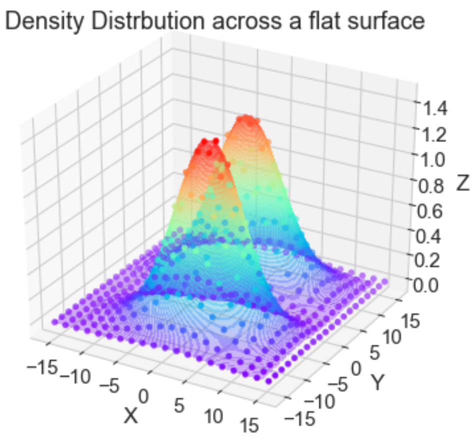
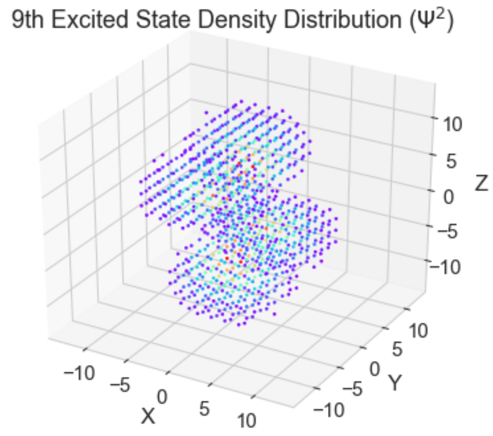
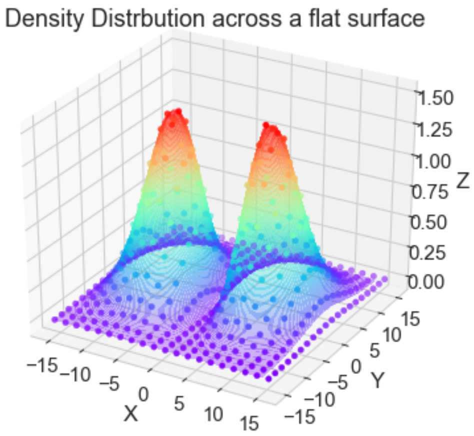
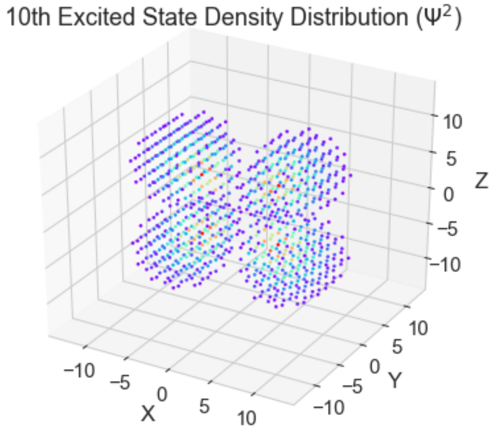

Density Distrbution across a flat surface

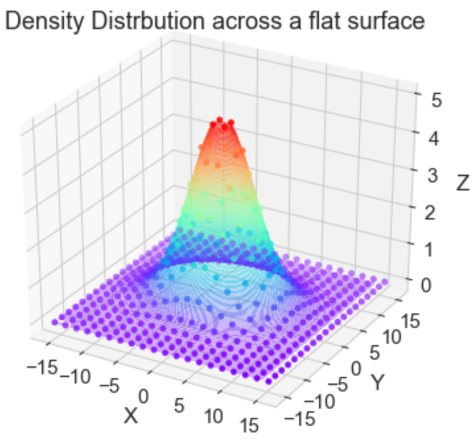

8th Excited State Density Distribution (Ψ^2)

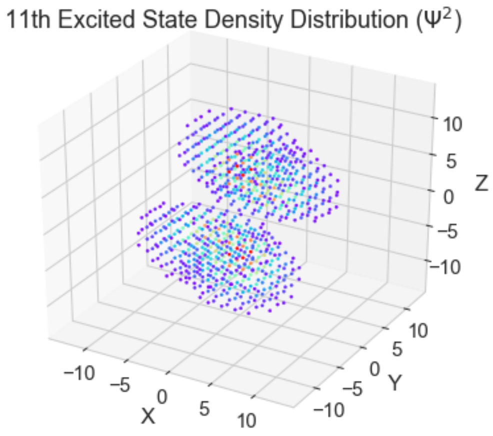

Density Distrbution across a flat surface
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Z
−15
−10
−5
0
5
10
15
X
15
10
5
0
−5
−10
−15
Y

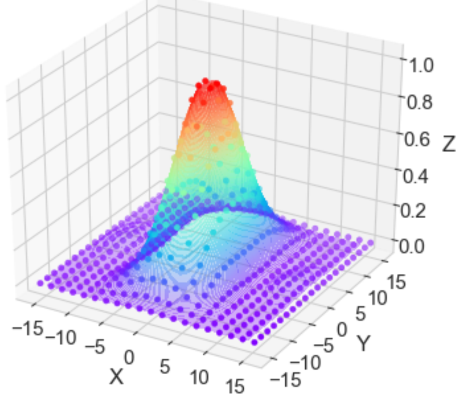

9th Excited State Density Distribution (Ψ^2)
10
5
0
−5
−10
Z
−10
−5
0
5
10
X
10
5
0
−5
−10
Y


Density Distrbution across a flat surface
1.50
1.25
1.00
0.75
0.50
0.25
0.00
Z
−15
−10
−5
0
5
10
15
X
15
10
5
0
−5
−10
−15
Y

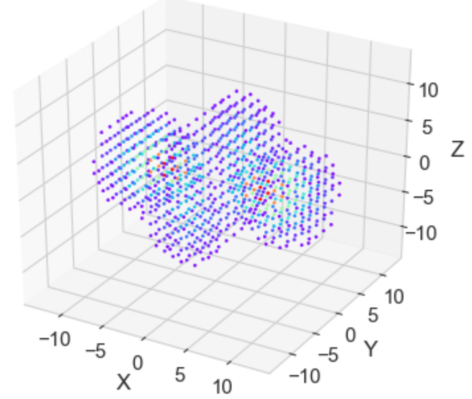

10th Excited State Density Distribution (Ψ^2)
10
5
0
−5
−10
Z
−10
−5
0
5
10
X
10
5
0
−5
−10
Y


Density Distrbution across a flat surface
5
4
3
2
1
0
Z
−15
−10
−5
0
5
10
15
X
15
10
5
0
−5
−10
−15
Y

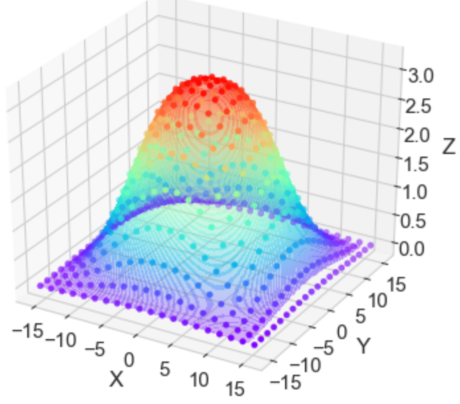

11th Excited State Density Distribution (Ψ^2)
10
5
0
−5
−10
Z
−10
−5
0
5
10
X
10
5
0
−5
−10
Y



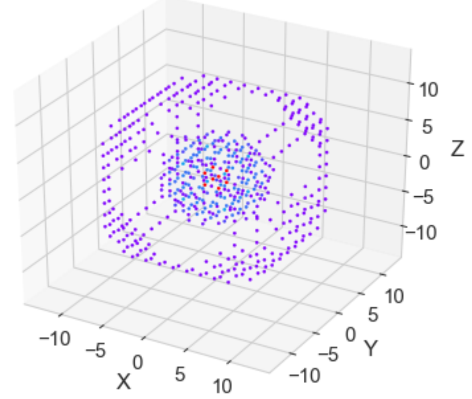
Density Distrbution across a flat surface



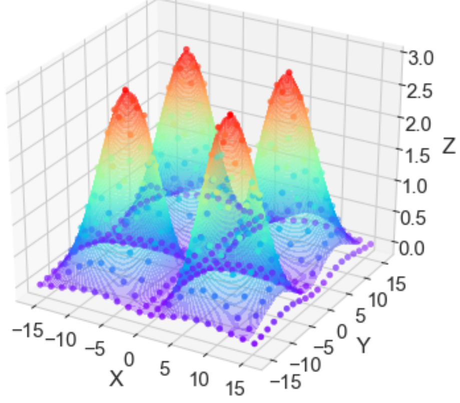
12th Excited State Density Distribution (Ψ^2)



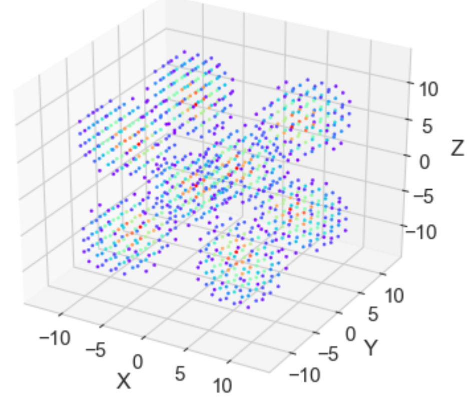
Density Distrbution across a flat surface



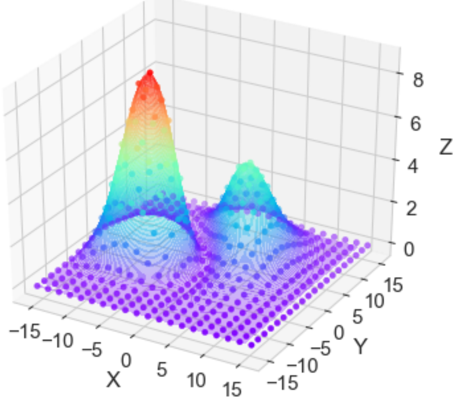
13th Excited State Density Distribution (Ψ^2)

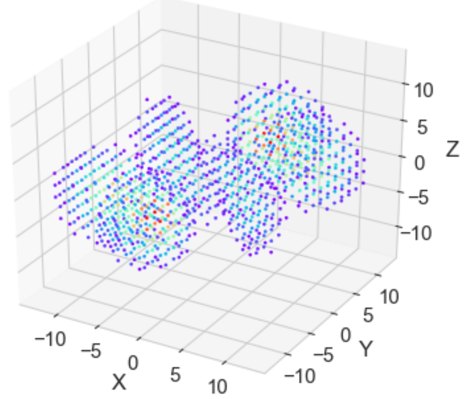


Density Distrbution across a flat surface



14th Excited State Density Distribution (Ψ^2)


Density Distrbution across a flat surface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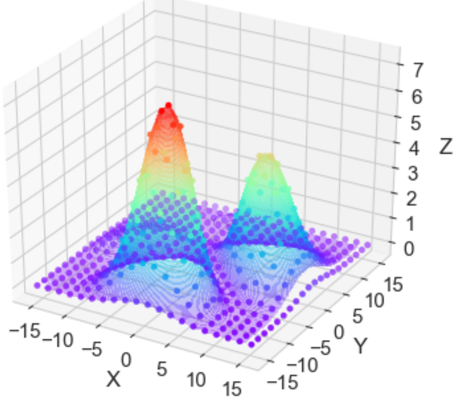
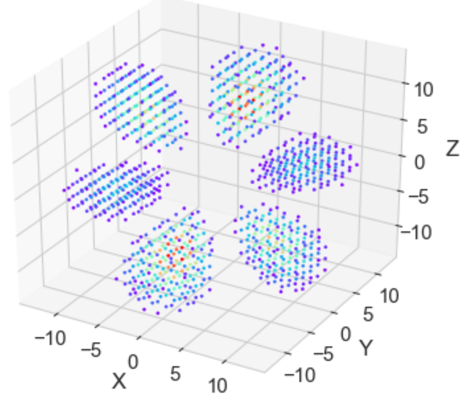
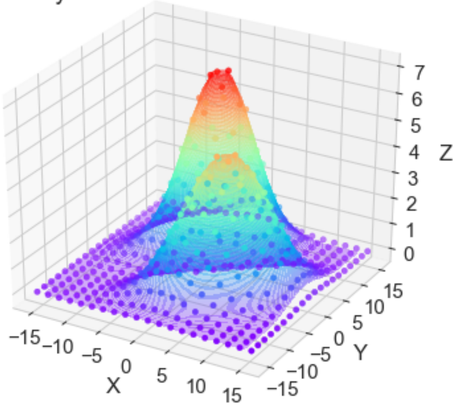
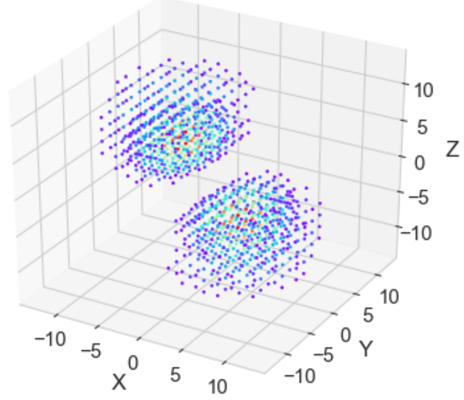
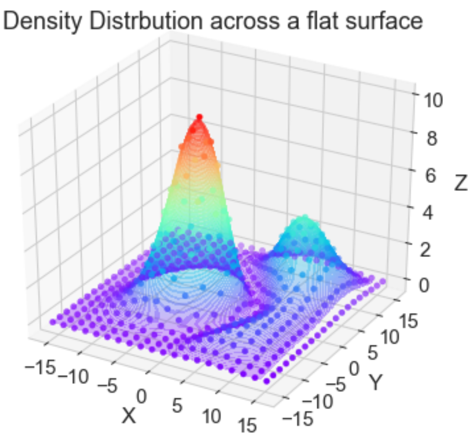
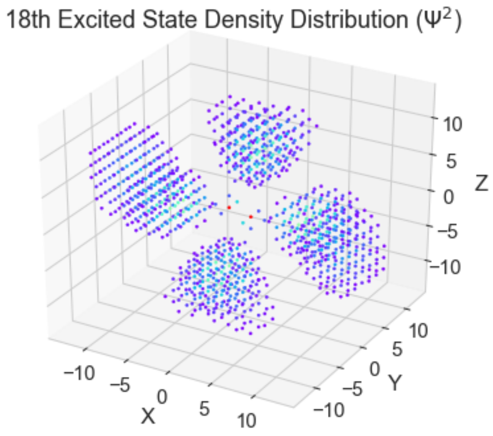

Density Distrbution across a flat surface

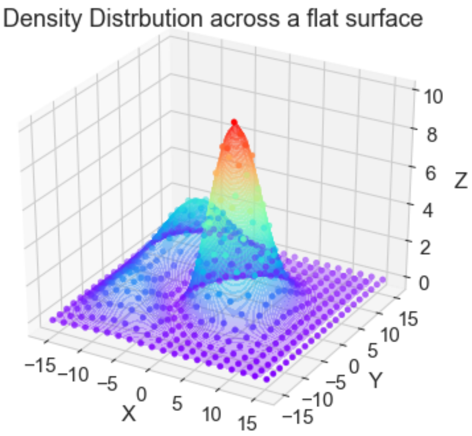

16th Excited State Density Distribution (Ψ^2)

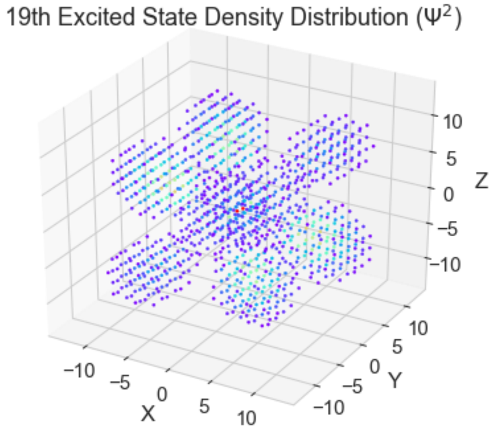

Density Distrbution across a flat surface


17th Excited State Density Distribution (Ψ^2)


Density Distrbution across a flat surface


18th Excited State Density Distribution (Ψ^2)


Density Distrbution across a flat surface


19th Excited State Density Distribution (Ψ^2)