In [ ]:
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Plotting Hydrogen orbitals for different values of n,l & m
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In [4]:
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import warnings
warnings.filterwarnings('ignore')
import numpy
import math
import matplotlib.pyplot as plt
from matplotlib.widgets import Slider, Button, RadioButtons
import scipy.special
from scipy.special import sph_harm
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import cm
from matplotlib.colors import ListedColormap
import skimage
from skimage import measure

def hydrogen_wf(n,l,m,X,Y,Z):
    R = numpy.sqrt(X**2+Y**2+Z**2)
    Theta = numpy.arccos(Z/R)
    Phi = numpy.arctan2(Y,X)

    rho = 2.*R/n
    s_harm=sph_harm(m, l, Phi, Theta)
    l_poly = scipy.special.genlaguerre(n-l-1,2*l+1)(rho)

    prefactor = numpy.sqrt((2./n)**3*math.factorial(n-l-1)/(2.*n*math.factorial(n+l)))
    wf = prefactor*numpy.exp(-rho/2.)*rho**l*s_harm*l_poly
    wf = numpy.nan_to_num(wf)
    return wf

dz=0.5
zmin=-10
zmax=10
x = numpy.arange(zmin,zmax,dz)
y = numpy.arange(zmin,zmax,dz)
z = numpy.arange(zmin,zmax,dz)
X,Y,Z = numpy.meshgrid(x,y,z) #X, Y, Z are 3d arrays that tell us the values of x, y, and z at every point in space

orbitals = [[1,0,0], [2,0,0], [3,1,0], [4,0,0], [4,1,0], [4,2,0], [4,3,0]]
for i in orbitals:
    n=i[0]
    l=i[1]
    m=i[2]
    data = hydrogen_wf(n,l,m,X,Y,Z)
    data = abs(data)**2
    R = numpy.sqrt(X**2+Y**2+Z**2)

    fig = plt.figure()
    ax = fig.add_subplot(111, projection='3d')
    ax.set_xlim([0,len(x)])
    ax.set_ylim([0,len(y)])
    ax.set_zlim([0,len(z)])
    max_val = numpy.max(data)

    verts, faces, _, _ = measure.marching_cubes(data, max_val/2, spacing = (1,1,1))
    result=ax.plot_trisurf(verts[:,0], verts[:,1], faces, verts[:,2], cmap ='Spectral', lw=0)

    ax.set_title("Hydrogen Orbital : n="+str(n)+", l="+str(l)+", m="+str(m))

    plt.show()
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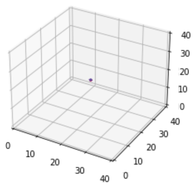
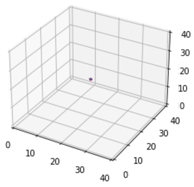
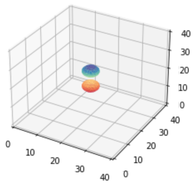
Hydrogen Orbital : n=1, l=0, m=0



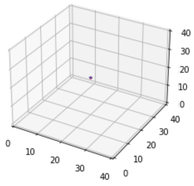
Hydrogen Orbital : n=2, l=0, m=0



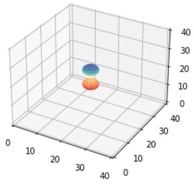
Hydrogen Orbital : n=3, l=1, m=0



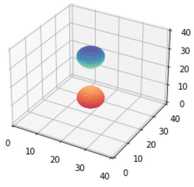
Hydrogen Orbital : n=4, l=0, m=0



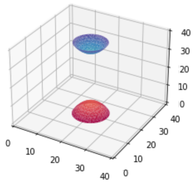
Hydrogen Orbital : n=4, l=1, m=0



Hydrogen Orbital : n=4, l=2, m=0



Hydrogen Orbital : n=4, l=3, m=0



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