

```

function hAtomAngular()
%Function written by Hew, Justin Kin Jun
%Started on 4th November 2020, Completed on 6th
%Written for computational MATLAB assignment for PHYS2150: Methods in
%Physics I
%Computed spherical harmonics using legendre function as well as its norm
%squared value
%Considered that the legendre function does not work for -ve values, a
%different function was inputted in its stead for different m values.
%Any input of l,m,n that fits the conditions described below will display
%the following: a 3d surface of the angular probability density function,
%and the polar plot of the function against theta

l= input('value of l:');
m= input('value of m:');
n= input('value of n:');
if (l < n) && (-1 <= m) && (m <= l) %conditions as described in paper
    disp ('valid')
else
    disp ('invalid')
    return
end

if isinteger(l)
    disp('valid') %Angular Quantum Number should be an integer, isinteger function ✓
was used because there is problems with the mod function
elseif mod(l,1) ~= 0
    disp('invalid')
    return
end

%I have included some integer conditions for input values but this is not
%necessary. The Reshape function can be adjusted such that it only works for ✓
integers.

%Establish a linear space with spherical coordinate system
if m > 0
dx = pi/240;
alt = -pi:dx:pi;
az = 0:dx:2*pi;
[phi,theta] = meshgrid(az,alt);
Plm= legendre(l,cos(theta));
P32 = reshape(Plm(m+1,:,:), size(phi));
a = (2*l+1)*factorial(l-m);
b = 4*pi*factorial(l+m);
C = sqrt(a/b);
Y = abs(C .* P32 .* exp(1i*m*phi)).^2;
[Xm,Ym,Zm] = sph2cart(phi, theta, (Y));
title('Probability Density','interpreter','latex');
figure (1)
surf(Xm,Ym,Zm);

elseif m==0 && l~=0 %ran into some problems with reshape function for m=0, also l=0 ✓

```

```

requires different case
dx = pi/240;
alt = -pi:dx:pi;
az = 0:dx:2*pi;
[phi,theta] = meshgrid(az,alt);
Plm= legendre(l,cos(theta));
P32 = reshape(Plm(m+1,:,:), size(phi));
a = (2*l+1);
b = 4*pi;
C = sqrt(a/b);
Y = abs(C .* P32).^2;
[Xm,Ym,Zm] = sph2cart(phi, theta, real(Y));
figure (1)
surf(Xm,Ym,Zm);
title('Probability Density','interpreter','latex');
elseif (m < 0)
m = -m;
dx = pi/240;
alt = -pi:dx:pi;
az = 0:dx:2*pi;
[phi,theta] = meshgrid(az,alt);
P= legendre(l,cos(theta));
a = (2*l+1)*factorial(l-m);
b = 4*pi*factorial(l+m);
C = sqrt(a/b);
P32 = reshape(P(m+1,:,:), size(phi));
Y = abs((factorial(l-m)./factorial(l+m)).*C.*(-1).^m.*P32).^2; %plugging hint and
using it
[Xm,Ym,Zm] = sph2cart(phi, theta, (Y));
figure (1)
surf(Xm,Ym,Zm);
title('Probability Density ','interpreter','latex');
elseif l==0 %ran into problems with l=0 so extended here
    dx = pi/240;
    alt = -pi:dx:pi;
    az = 0:dx:2*pi;
    [phi,theta] = meshgrid(az,alt);
    Plm= legendre(l,cos(theta));
    P32 = reshape(Plm(), size(phi));
    a = (2*l+1);
    b = 4*pi;
    C = sqrt(a/b);
    Y = abs(C .* P32).^2;
    [Xm,Ym,Zm] = sph2cart(phi, theta, real(Y));
    figure (1)
    surf(Xm,Ym,Zm);
    title('Probability Density','interpreter','latex');
end
figure (2)
polarplot(theta(:,2),Y(:,2)) %choose an arbitrary number on the surface
end

```

%This is an additional segment which shows the code for the evaluation of

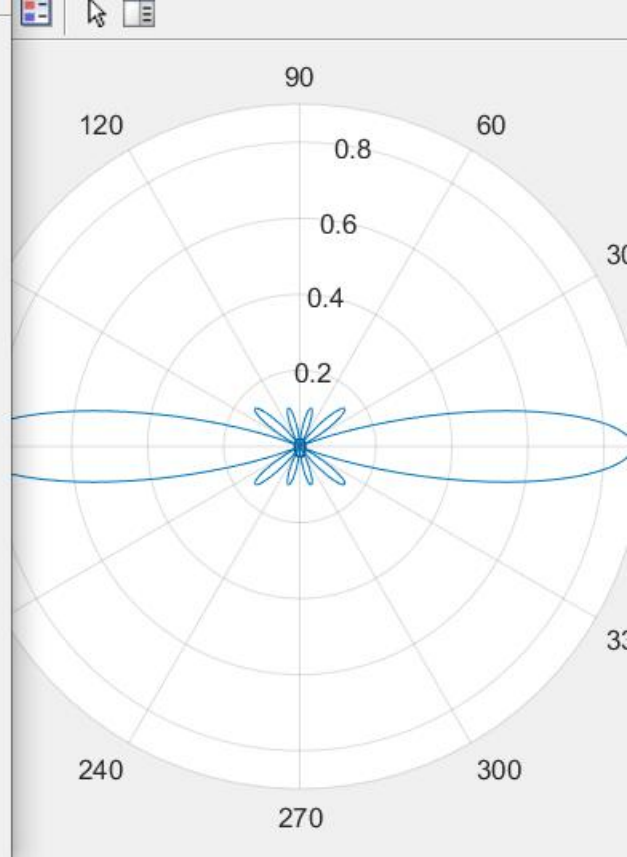
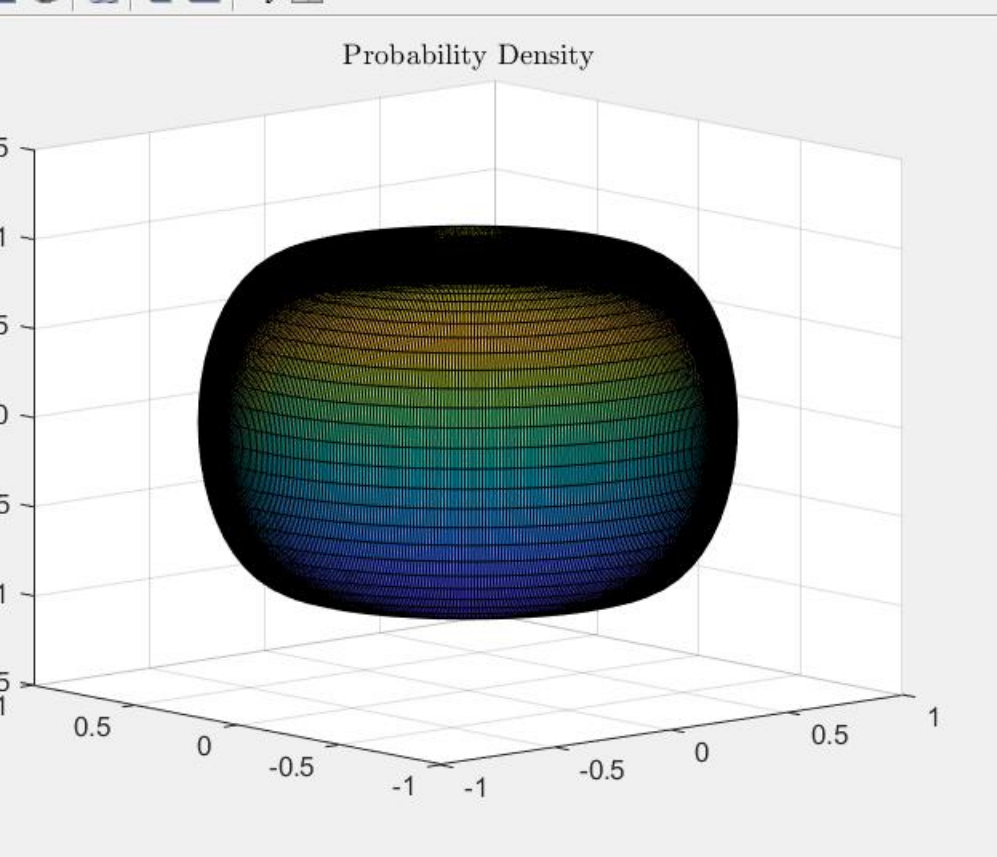
```
%the legendre function for spherical harmonics; to answer part b of the
%homework sheet
%I tried to use a nested function but it seemed not to work, an anonymous
%function is used instead so a file is not created
%This function is not used as the spherical harmonics is already computed
%in the prior code
```

```
function SphHarmonic()
```

```
l= input('value of l:');
m= input('value of m:');
n= input('value of n:');
dx = pi/60;
alt = -pi:dx:pi;
az = 0:dx:2*pi;
[phi,theta] = meshgrid(az,alt);
s = @(m,n,l) legendre(l,cos(theta));
P32 = reshape(s(m+1,:,:), size(phi));
a = (2*l+1)*factorial(l-m);
b = 4*pi*factorial(l+m);
C = sqrt(a/b);
Y = (C .* P32 .* exp(1i*m*phi));
[~,~,~] = sph2cart(phi, theta,real(Y));
title('Spherical Harmonics','interpreter','latex');
figure (3)
surf(Xm,Ym,Zm);
end
```

```
    %Matlab documentation for the legendre function was used as reference
```

```
% disp(a);
% disp(b);
% disp(C);
```



function for $m=0$, also 1

Details

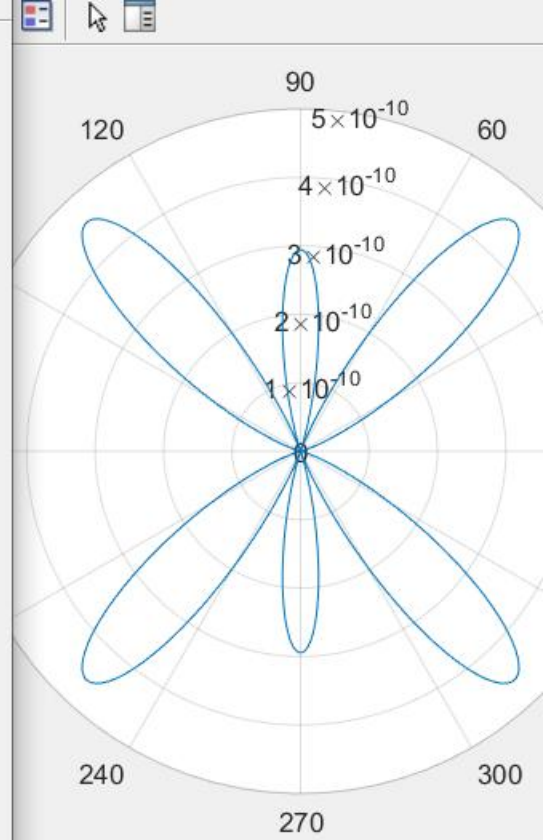
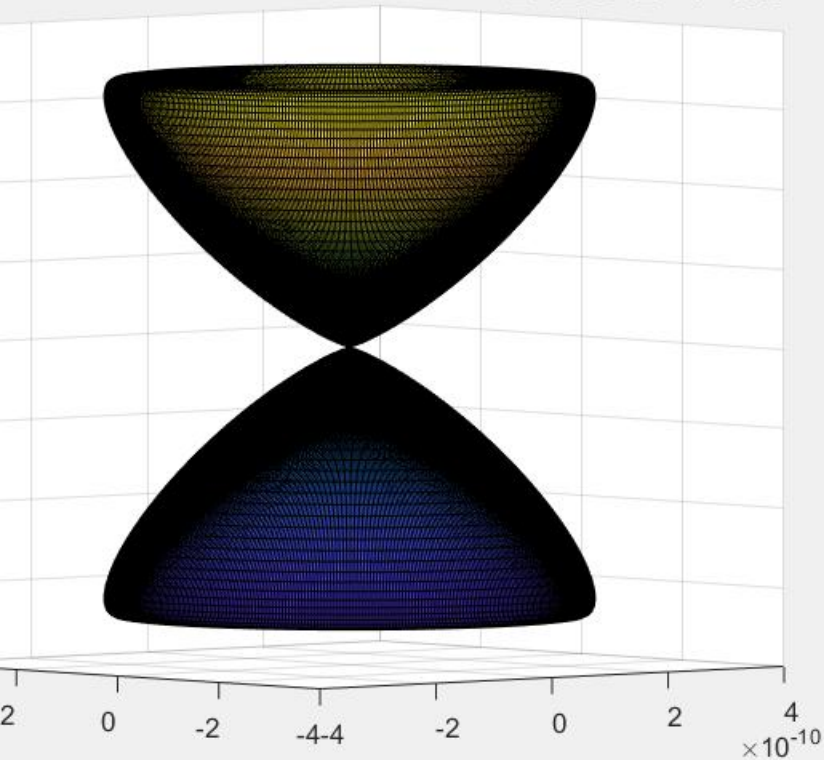
Select a file to view details

```
value of n:6  
valid  
>> hAtomAngular  
value of l:5  
value of m:-3  
value of n:6  
valid  
>> hAtomAngular  
value of l:5  
value of m:0  
value of n:6  
valid
```

f_x >>

<

Probability Density

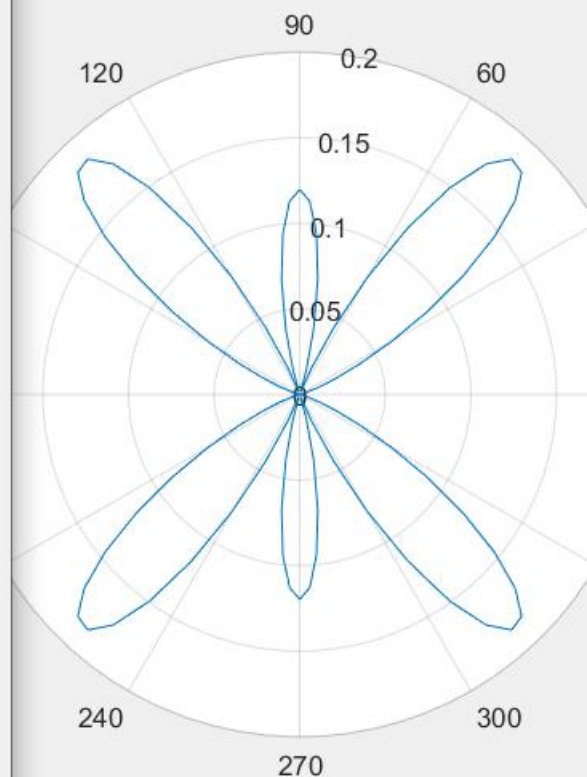
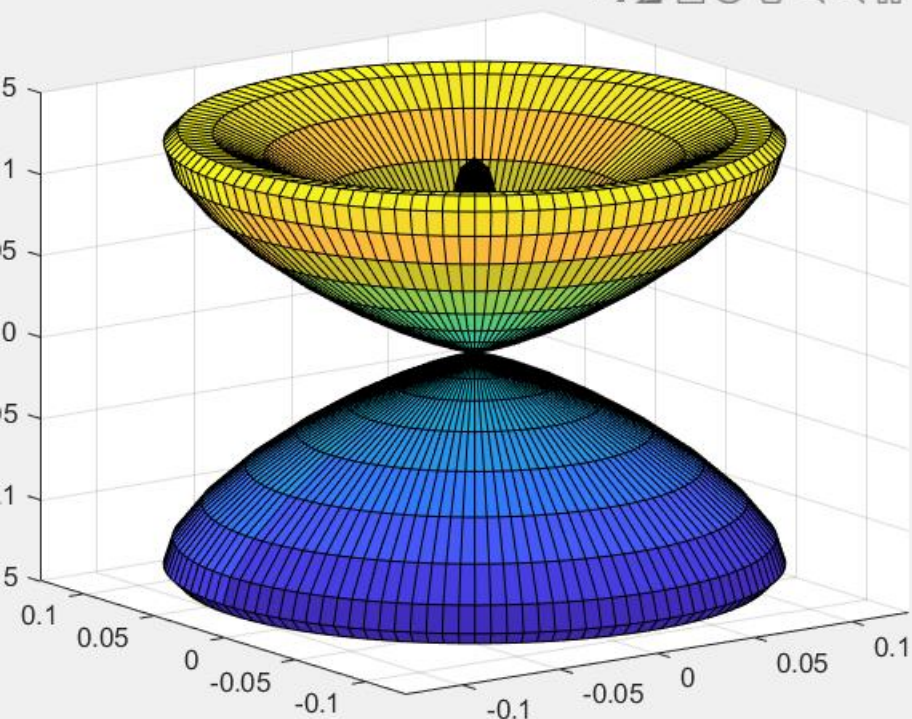


for m=0, also 1:

Details

Select a file to view details

```
value of n:6
valid
>> hAtomAngular
value of l:5
value of m:3
value of n:6
valid
>> hAtomAngular
value of l:5
value of m:-3
value of n:6
valid
fx >>
<
```



ed as reference

Details

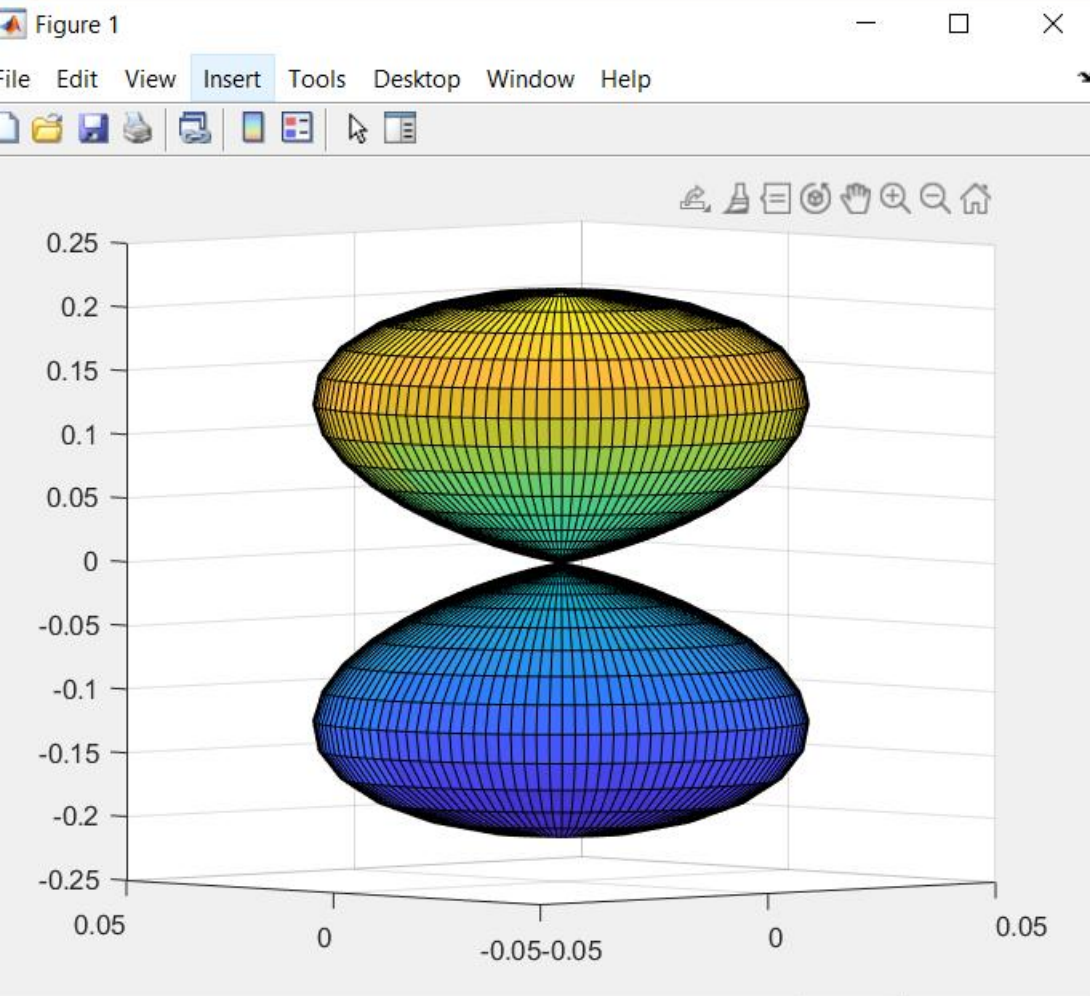
Select a file to view details

```
value of n:7
invalid
>> hAtomAngular
value of l:5
value of m:5
value of n:7
valid
>> hAtomAngular
value of l:5
value of m:3
value of n:6
valid
```

fx >>

<

>



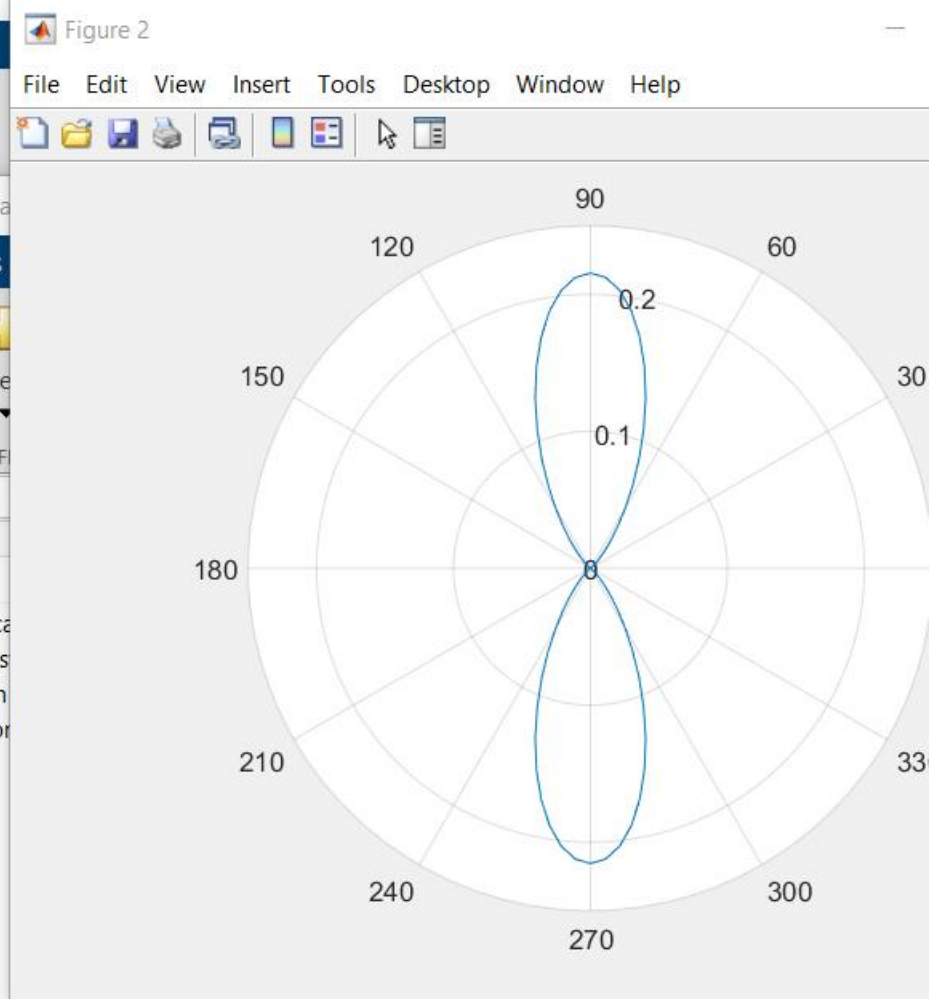
Quantum Number should be an integer, isinteger function

integer conditions for input values but this is not
function can be adjusted such that it only works for inte

with spherical coordinate system

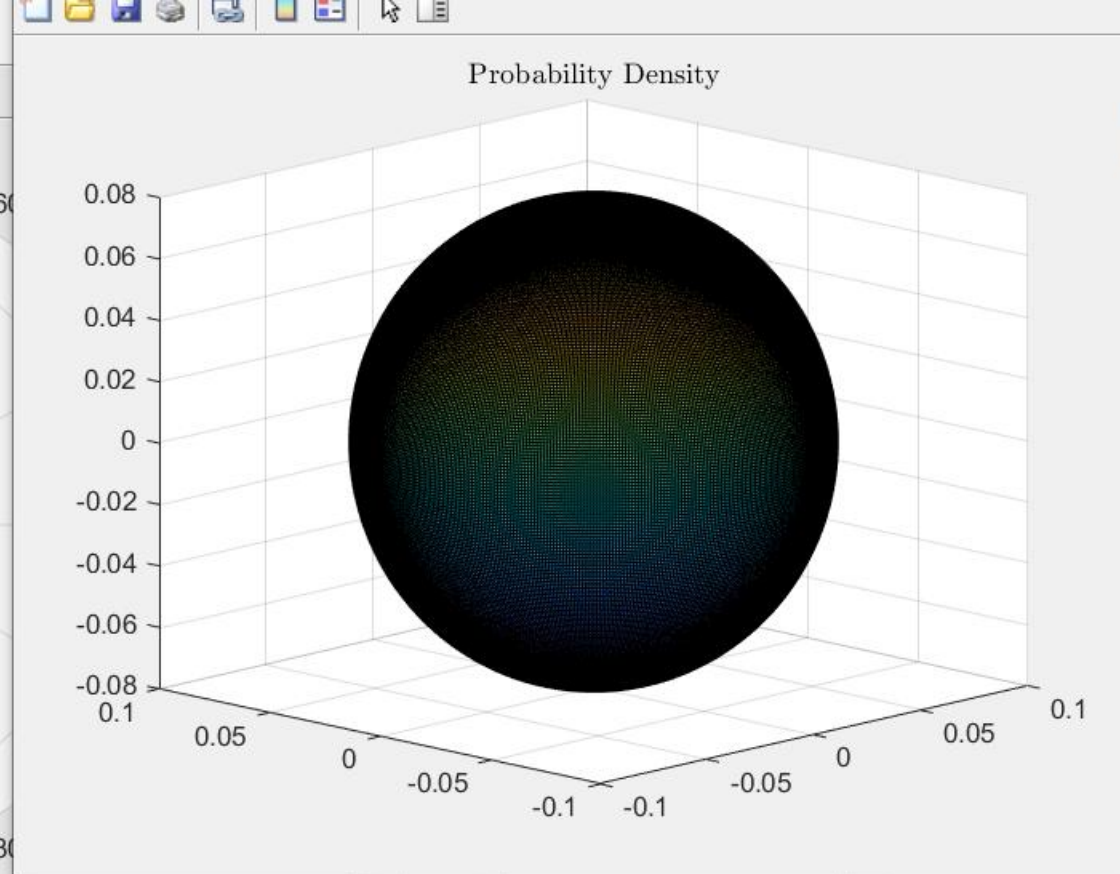
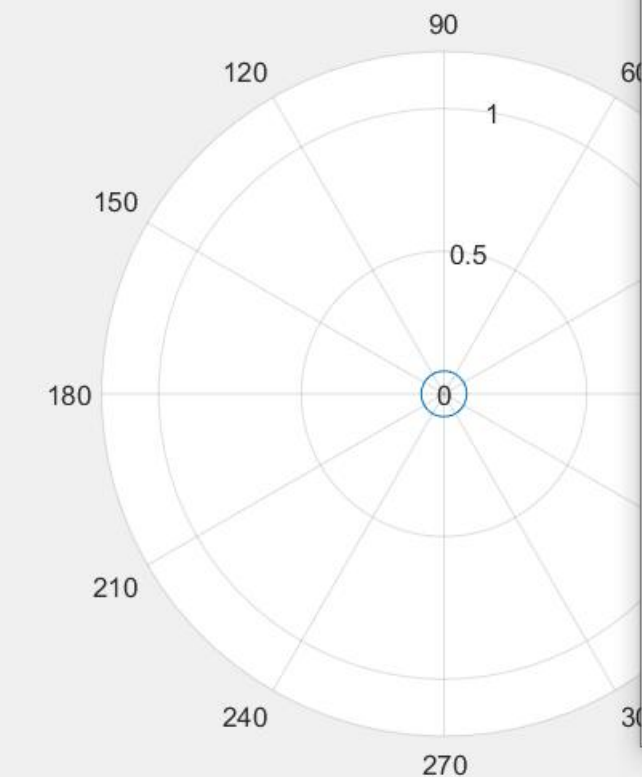
Details

Select a file to view details



```
value of n:1
valid
>> hAtomAngular
value of l:5
value of m:6
value of n:7
invalid
>> hAtomAngular
value of l:5
value of m:5
value of n:7
valid
```

fx >>



```
valid') %Angular Quantum Number should be an integer,isinteger function
(1,1) ~= 0
invalid')
```

cluded some integer conditions for input values but this is not
The Reshape function can be adjusted such that it only works for inte

a linear space with spherical coordinate system

```
dx:pi;
*pi;
= meshgrid(az,alt):
```

Details

Select a file to view details

```
value of n:6
valid
>> hAtomAngular
value of l:0
value of m:0
value of n:1
valid
>> hAtomAngular
value of l:0
value of m:0
value of n:1
valid
fx >>
<
```