# 第三次作业

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# 缔合拉盖尔多项式

$$L_k^p(t)=(-1)^prac{d^p}{dt^p}L_{k+p}(t)$$

己知

$$L_n(x)=rac{e^x}{n!}rac{d}{dx^n}(x^ne^{-x})$$

容易推出: 
$$L_{n+1}(x) = (2n+1-x)L_n(x) - n^2L_{n-1}(x)$$

$$L_0(x) = 1$$

$$L_1(x) = -x + 1$$

$$L_2(x) = x^2 - 4x + 2$$

进行扩展

$$L_k^p(t)=(-1)^prac{d^p}{dt^p}L_{k+p}(t)$$

类比p=0,将L表达式代入,容易推出:

$$L_{k+1}^p(x) = rac{2k+1+p-x}{k+1}L_k^p(x) - rac{p+k}{k+1}L_{k-1}^p(x)$$

$$L_0^p(x) = 1$$

$$L_1^p(x) = -x + p + 1$$

$$L_2^p(x) = rac{1}{2}[x^2 - 2(k+2)x + (k+1)(k+2)]$$

```
import pandas as pd
import sympy as sy

def Laguerre(k,p):
    L0p=1
    L1p=-x+p+1
    L2p=1/2*(x**2-2*(p+2)*x+(p+1)*(p+2))
    if k==0:
        return L0p
    elif k==1:
        return L1p
    elif k==2:
        return L2p
    elif k>2:
        temp=(2*k-1-x)/k*Laguerre(k-1,p)-(k-1)/k*Laguerre(k-2,p)
        return temp
```

```
import pandas as pd
import sympy as sy
x= sy.symbols("x")
data_df = pd.DataFrame()
data_df['n'] = range(0,6)
data_df['11'] = [0,0,0,1,0,1]
data_df['L(1+1/2,(n-1)/2)(x)0']=
[Laguerre(0,1/2), Laguerre(0,3/2), Laguerre(1,1/2), Laguerre(1,3/2), La
guerre(2,1/2), Laguerre(2,3/2)
data_df['12']=[None, None, 2, 3, 2, 3]
data_df['L(1+1/2,(n-1)/2)(x)1']=
[None, None, Laguerre(0, 3/2), Laguerre(0, 5/2), Laguerre(1, 5/2), Laguerre
(1,7/2)
data_df['13']=[None, None, None, None, 4, 5]
data_df['L(1+1/2,(n-1)/2)(x)2']=
[None, None, None, Laguerre(0, 9/2), Laguerre(0, 11/2)]
data_df
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	N	L1	L(L+1/2,(N-L)/2)(X)0	L2	L(L+1/2,(N-L)/2) (X)1	L3	L(L+1/2,(N-L)/2) (X)2
0	0	0	1	NaN	None	NaN	NaN
1	1	0	1	NaN	None	NaN	NaN
2	2	0	1.5 - x	2.0	1	NaN	NaN
3	3	1	2.5 - x	3.0	1	NaN	NaN
4	4	0	0.5*x**2 - 2.5*x + 1.875	2.0	3.5 - x	4.0	1.0
5	5	1	0.5*x**2 - 3.5*x + 4.375	3.0	4.5 - x	5.0	1.0

与table4-5进行对比,结果一模一样,没有问题下面进行画图分析

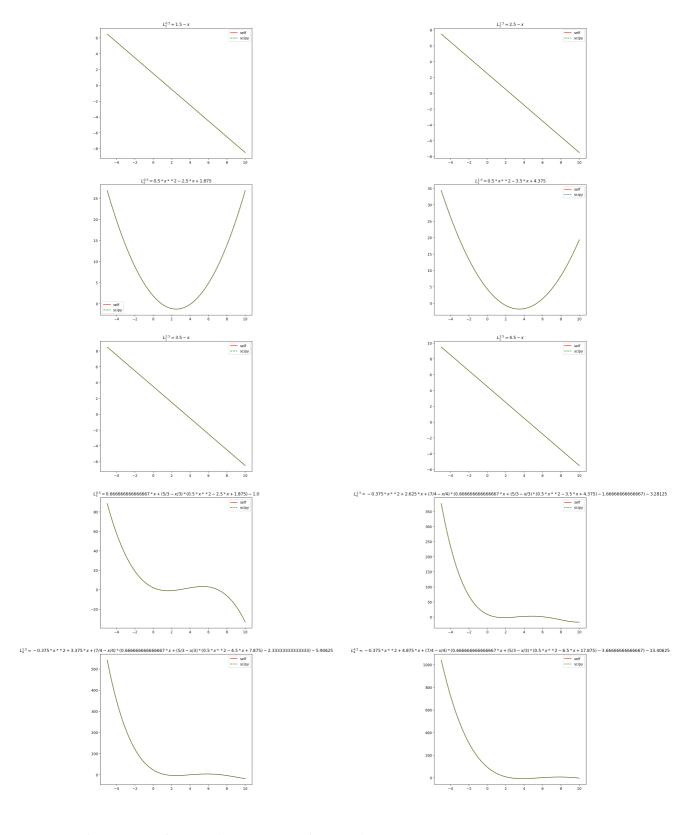
```
import sympy as sy
x=sy.symbols('x')
def Laguerre_shuzhi(x,k,p):#数值运算
    L0p=1
    L1p=-x+p+1
    L2p=1/2*(x**2-2*(p+2)*x+(p+1)*(p+2))
    if k=0:
        return L0p
    elif k==1:
        return L1p
    elif k==2:
        return L2p
    elif k>2:
        temp=(2*k-1+p-x)/k*Laguerre_shuzhi(x,k-1,p)-(k-1+p)/k*Laguerre_shuzhi(x,k-2,p)
        return temp
```

# 画图分析 与scipy进行比较分析

```
import matplotlib.pyplot as plt
import numpy as np
import scipy.special as special

plt.figure(figsize=(25,40),dpi=200)
klist=[1,1,2,2,1,1,3,4,4,4]
plist=[1/2,3/2,1/2,3/2,5/2,7/2,1/2,3/2,5/2,9/2]
for i in range(1,11):
    plt.subplot(5,2,i)
    k=klist[i-1]
    p=plist[i-1]
    title=Laguerre(k,p)
    plt.title('$L_{}^{s_{-}}$'.format(k,{p},title))
    plt.subplots_adjust(left=None, bottom=None, right=None, top=None, wspace=1.2,
hspace=None)
    ff=np.linspace(-5,10,200)
```

```
ylist=[]
ytrue=[]
for j in range(0,len(ff)):
    temp1=ff[j]
    yy1=Laguerre_shuzhi(temp1,k,p)
    yy2=special.assoc_laguerre(temp1,k,p)
    ylist.append(yy1)
    ytrue.append(yy2)
plt.plot(ff,ylist,'r',label='self')
plt.plot(ff,ytrue,'g',label='scipy',linestyle='dashed')
plt.legend()
```



由绘制的图像可知,自己编写的拉盖尔多项式与sci库几乎完全重合

# 氢原子相关

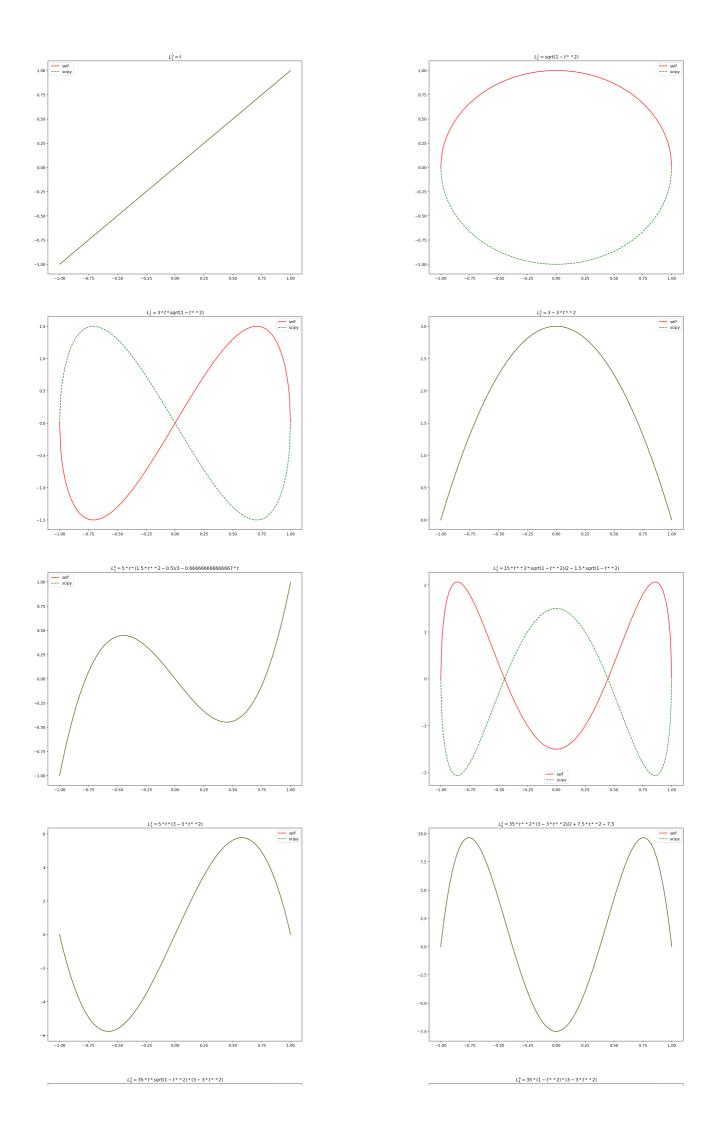
# 关联勒让德函数

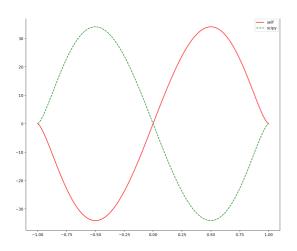
```
import pandas as pd
import sympy as sy
t=sy.symbols("t")
def Legendre(t,1,m):
    if m==0:
        L0m=1
        L1m=t
        L2m=1/2*(3*t**2-1)
    elif abs(m)==1:
        LOm=0
        L1m=sy.sqrt(1-t**2)
        L2m=3*sy.sqrt(1-t**2)*t
    elif abs(m)==2:
        L0m=0
        L1m=0
        L2m=3*(1-t**2)
    else:
        L0m=0
        L1m=0
        L2m=0
    if 1==0:
        return LOm
    elif l==1:
        return L1m
    elif 1==2:
        return L2m
    elif 1>2 and (1-m)!=0:
        temp=(2*1-1)*t/(1-m)*Legendre(t,1-1,m)-(1-1+m)/(1-m)*Legendre(t,1-2,m)
        return temp
    elif 1>2 and (1-m)==0:
        temp=Legendre(t, l-2, m)+(2*l-1)*sy.sqrt(l-t**2)*Legendre(t, l-1, m-1)
        return temp
```

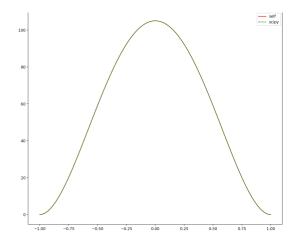
```
def Legendre_shuzhi(t,1,m):
    if m==0:
        L0m=1
        L1m=t
        L2m=1/2*(3*t**2-1)
    elif abs(m)==1:
        L0m=0
        L1m=sy.sqrt(1-t**2)
        L2m=3*sy.sqrt(1-t**2)*t
    elif abs(m)==2:
        L0m=0
        L1m=0
        L2m=3*(1-t**2)
    else:
```

```
L0m=0
                                                              L1m=0
                                                            L2m=0
                               if 1==0:
                                                              return LOm
                               elif l==1:
                                                            return L1m
                               elif 1==2:
                                                          return L2m
                               elif 1>2 and (1-m)!=0:
                                                             temp=(2*l-1)*t/(l-m)*Legendre_shuzhi(t,l-1,m)-(l-1+m)/(l-1+m)
m)*Legendre_shuzhi(t,1-2,m)
                                                             return temp
                               elif 1>2 and (1-m)==0:
                                                            temp=Legendre\_shuzhi(t,l-2,m)+(2*l-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre\_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*Legendre_shuzhi(t,l-1,m-1)*sy.sqrt(1-t**2)*sy.sqrt(1-t**2)*sy.sqrt(1-t**2)*Legendre_shuzhi(t,l-1,m
1)
                                                              return temp
```

```
import matplotlib.pyplot as plt
import numpy as np
import scipy.special as special
plt.figure(figsize=(30,60),dpi=200)
klist=[1,1,2,2,3,3,3,4,4,4]
plist=[0,1,1,2,0,1,2,2,3,4]
for i in range(1,11):
    plt.subplot(5,2,i)
    l=klist[i-1]
    m=plist[i-1]
    t=sy.symbols('t')
    title=Legendre(t,1,m)
    plt.title('$L_{}^{}={}$'.format(1,{m},title))
    plt.subplots_adjust(left=None, bottom=None, right=None, top=None, wspace=0.5,
hspace=None)
    ff=np.linspace(-1,1,200)
    ylist=[]
    ytrue=[]
    for j in range(0,len(ff)):
        temp1=ff[j]
        yy1=Legendre_shuzhi(temp1,1,m)
        yy2=special.lpmv(m,1,temp1)
        ylist.append(yy1)
        ytrue.append(yy2)
    plt.plot(ff,ylist,'r',label='self')
    plt.plot(ff,ytrue,'g',label='scipy',linestyle='dashed')
    plt.legend()
```







可以看到, 部分值由于初始设置的正负而产生了正反差异

#### 球谐函数

```
def Ball(l,m):
    j1=sy.symbols('j1')
    j2=sy.symbols('j2')
    if m>=0:
        epsi=(-1)**m
    else:
        epsi=1
    YY=epsi*np.sqrt((2*l+1)*np.math.factorial(l-
abs(m))/4/np.pi/np.math.factorial(l+abs(m)))*sy.exp(1j*m*j1)*Legendre(sy.cos(j2),l,m)
    return YY
```

#### Ball(3,2)

 $0.340661825477761\left(3 - 3\cos^2{(j_2)}\right)e^{2.0ij_1}\cos{(j_2)}$ 

与量子力学课本形式一致

## 推导

氢原子的势能 $V\left(r
ight)=-rac{e^{2}}{4\piarepsilon_{0}}rac{1}{r}$ 

径向方程: 
$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 u}{\mathrm{d}r^2} + [-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}]u = uE$$

首先需要对形式进行简化

$$\kappa \equiv rac{\sqrt{-2mE}}{\hbar}$$

引入
$$ho\equiv\kappa r$$
和 $ho_0\equivrac{me^2}{2\piarepsilon_0\hbar^2\kappa}$ 

这样经过化简可以得到

$$rac{\mathrm{d}^2 u}{\mathrm{d}
ho^2} = [1 - rac{
ho_0}{
ho} + rac{l(l+1)}{
ho^2}]u$$

分别在 $\rho \to \infty$  和  $\rho \to 0$ 下进行考察

对 $\rho$ 较大时,有 $u(\rho) \approx A \exp(-\rho)$ 

对 $\rho$ 较小时,有 $u(\rho) \approx C \rho^{l+1}$ 

引入新的函数 $v(\rho)$ 

$$u(
ho)=
ho^{l+1}e^{-
ho}v(
ho)$$

 $v(\rho)$ 可以展开为幂级数,确定系数,逐项求导

化简可以由递推关系得到

$$v(
ho)=c_0e^{2
ho}$$

为了级数截断  $c_{(imax+1)} = 0$ 

主量子数 $n \equiv jmax + l + 1$ 

 $\rho_0 = 2n$ 

$$E=rac{-\hbar^2\kappa^2}{2m}$$

径向波函数:  $R_{nl}(r) = \frac{1}{r} \rho^{l+1} e^{-\rho} v(\rho)$ 

$$v(
ho) = L_{n-l-1}^{2l+1}(2
ho)$$

最终可以得到氢原子的归一化波函数为

$$\psi_{nlm} = \sqrt{(rac{2}{na})^3rac{(n-l-1)!}{2n[(n+l)!]^3}}e^{-r/na}(rac{2r}{na})^l[L_{n-l-1}^{2l+1}(2r/na)]Y_l^m( heta,\phi)$$

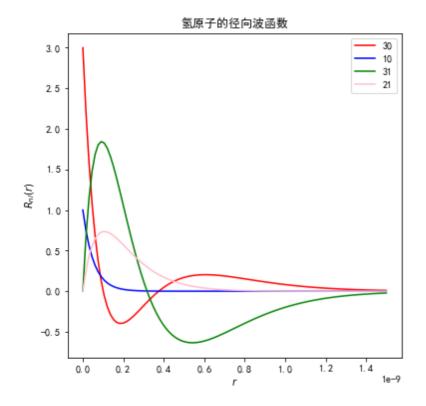
## 径向波函数绘制

```
def Rj(r,n,1):
    a0=0.529*10**(-10)
    p=r/a0/n
    v=Laguerre_shuzhi(2*p,n-1-1,2*1+1)
    R=(2*p)**(1)*np.exp(-p)*v
    return R
```

```
fig=plt.figure(figsize=(6,6))
Rlist1=np.linspace(0.0000001,1.5,100)
Rlist=[i*10**(-9) for i in Rlist1]
ylist1=[]
ylist2=[]
ylist3=[]
```

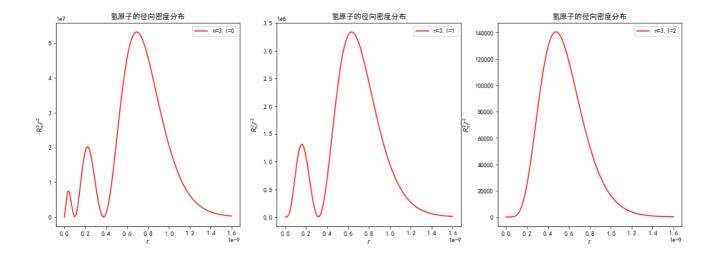
```
ylist4=[]
for i in range(0,len(Rlist)):
    temp=Rj(Rlist[i],3,0)
    ylist1.append(temp)
    temp1=Rj(Rlist[i],1,0)
    ylist2.append(temp1)
    temp2=Rj(Rlist[i],3,1)
    ylist3.append(temp2)
    temp3=Rj(Rlist[i],2,1)
    ylist4.append(temp3)
plt.plot(Rlist,ylist1,c='r',label='30')
plt.plot(Rlist,ylist2,c='b',label='10')
plt.plot(Rlist,ylist3,c='g',label='31')
plt.plot(Rlist,ylist4,c='pink',label='21')
plt.legend()
plt.rcParams['font.sans-serif']=['Simhei']
plt.rcParams['axes.unicode_minus']=False
plt.title("氢原子的径向波函数")
plt.ylabel('$R_{nl}(r)$')
plt.xlabel('$r$')
```

#### Text(0.5, 0, '\$r\$')

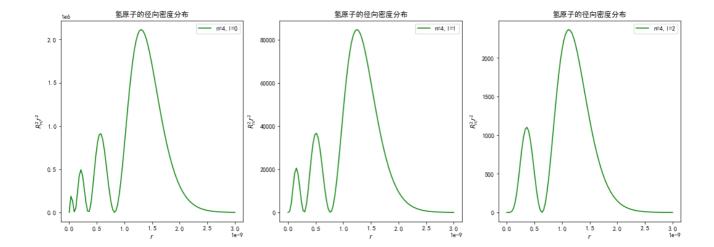


```
import math
def Rou(r,n,l):
    a=0.529*10**(-10)
    A=np.sqrt((2/n/a)**3*np.math.factorial(n-l-1)/2/n/(np.math.factorial(n+l))**3)
    #print('A',A)
    re=(Rj(r,n,l)*A*r)**2
    #print(Rj(r,n,l))
    return re
```

```
fig=plt.figure(figsize=(18,6))
Rlist1=np.linspace(0.0000001,1.6,100)
Rlist=[i*10**(-9) for i in Rlist1]
ylist1=[]
ylist2=[]
ylist3=[]
ylist4=[]
for i in range(0,len(Rlist)):
    temp=Rou(Rlist[i],3,0)
    ylist1.append(temp)
    temp2=Rou(Rlist[i],3,1)
    ylist3.append(temp2)
    temp3=Rou(Rlist[i],3,2)
    ylist4.append(temp3)
yresu=[ylist1,ylist3,ylist4]
nlist=[3,3,3]
11ist=[0,1,2]
for j in range(1,4):
    plt.subplot(1,3,j)
    plt.plot(Rlist,yresu[j-1],c='r',label='n=\{\},l=\{\}'.format(nlist[j-1],llist[j-1]))
    plt.legend()
    plt.rcParams['font.sans-serif']=['Simhei']
    plt.rcParams['axes.unicode_minus']=False
    plt.title("氢原子的径向密度分布")
    plt.ylabel('R_{nl}^2r^2$')
    plt.xlabel('$r$')
```



```
fig=plt.figure(figsize=(18,6))
Rlist1=np.linspace(0.0000001,3,100)
Rlist=[i*10**(-9) for i in Rlist1]
ylist1=[]
ylist2=[]
ylist3=[]
ylist4=[]
for i in range(0,len(Rlist)):
    temp=Rou(Rlist[i],4,0)
    ylist1.append(temp)
    temp2=Rou(Rlist[i],4,1)
    ylist3.append(temp2)
    temp3=Rou(Rlist[i],4,2)
    ylist4.append(temp3)
yresu=[ylist1,ylist3,ylist4]
nlist=[4,4,4]
11ist=[0,1,2]
for j in range(1,4):
    plt.subplot(1,3,j)
    plt.plot(Rlist,yresu[j-1],c='g',label='n=\{\},l=\{\}'.format(nlist[j-1],llist[j-1]))
    plt.legend()
    plt.rcParams['font.sans-serif']=['Simhei']
    plt.rcParams['axes.unicode_minus']=False
    plt.title("氢原子的径向密度分布")
    plt.ylabel('R_{nl}^2r^2')
    plt.xlabel('$r$')
```



## 角向分布

```
def Ball1(l,m,j1,j2):
    if m>=0:
        epsi=(-1)**m
    else:
        epsi=1
    YY=epsi*np.sqrt((2*l+1)*np.math.factorial(l-
abs(m))/4/np.pi/np.math.factorial(l+abs(m)))*
(np.cos(m*j1)+1j*np.sin(m*j1))*Legendre_shuzhi(np.cos(j2),l,m)
    return YY
```

```
test=Ball1(2,1,np.pi/2,np.pi/2)
print(test)
special.sph_harm(2, 1, np.pi/2, np.pi/2)
```

```
-2.89659256637091e-33 - 4.73049465100897e-17*I
```

```
(nan+0j)
```

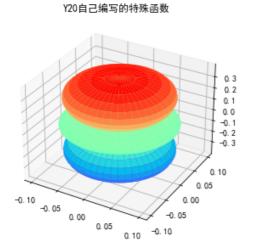
```
import numpy as np
import scipy.special
import matplotlib.pyplot as plt

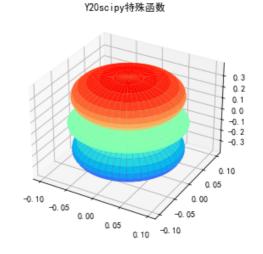
def sph(r, theta, phi):
    x = r * np.sin(theta) * np.cos(phi)
    y = r * np.sin(theta) * np.sin(phi)
    z = r * np.cos(theta)
    return np.array([x, y, z])
```

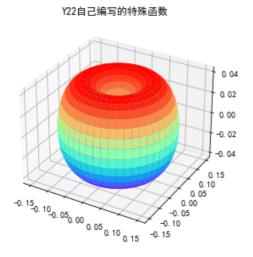
```
1 = 2
m = 0
Y]m=[]
num=100
theta = np.linspace(0, np.pi, num)
phi = np.linspace(0, 2 * np.pi, num)
Theta, Phi = np.meshgrid(theta, phi)
Ylm1 = Ball1(1, m, Phi, Theta)
for i in range(0,num):
    for j in range(0, num):
        Ylm1[i][j]=complex(Ylm1[i,j])
Y1m2 = np.abs(Y1m1)**2
X, Y, Z = sph(Ylm2, Theta, Phi)
plt.rcParams['font.sans-serif']=['Simhei']
plt.rcParams['axes.unicode_minus']=False
fig = plt.figure(figsize=(16,16))
ax = fig.add_subplot(3,2,1,projection = "3d")
ax.set_title("Y%d%d自己编写的特殊函数" % (1, m))
ax.plot_surface(X, Y, Z, cmap="rainbow")
1 = 2
m = 0
Y]m=[]
num=100
theta = np.linspace(0, np.pi, num)
phi = np.linspace(0, 2 * np.pi, num)
Theta, Phi = np.meshgrid(theta, phi)
Ylm = special.sph_harm(m, 1, Phi, Theta)
Ylm2 = np.abs(Ylm)**2
X, Y, Z = sph(Ylm2, Theta, Phi)
plt.rcParams['font.sans-serif']=['Simhei']
plt.rcParams['axes.unicode_minus']=False
ax = fig.add_subplot(3,2,2,projection = "3d")
ax.set_title("Y%d%dscipy特殊函数" % (1, m))
ax.plot_surface(X, Y, Z, cmap="rainbow")
1 = 2
m = 2
Y]m=[]
num=100
theta = np.linspace(0, np.pi, num)
phi = np.linspace(0, 2 * np.pi, num)
Theta, Phi = np.meshgrid(theta, phi)
Ylm1 = Ball1(1, m, Phi, Theta)
for i in range(0, num):
    for j in range(0, num):
        Ylm1[i][j]=complex(Ylm1[i,j])
Y1m2 = np.abs(Y1m1)**2
X, Y, Z = sph(Ylm2, Theta, Phi)
plt.rcParams['font.sans-serif']=['Simhei']
```

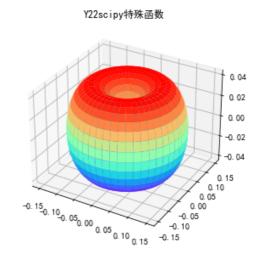
```
plt.rcParams['axes.unicode_minus']=False
fig = plt.figure(figsize=(16,16))
ax = fig.add_subplot(3,2,3,projection = "3d")
ax.set_title("Y%d%d自己编写的特殊函数" % (1, m))
ax.plot_surface(X, Y, Z, cmap="rainbow")
1 = 2
m = 2
Y1m=[]
num=100
theta = np.linspace(0, np.pi, num)
phi = np.linspace(0, 2 * np.pi, num)
Theta, Phi = np.meshgrid(theta, phi)
Ylm = special.sph_harm(m, 1, Phi, Theta)
Y1m2 = np.abs(Y1m)**2
X, Y, Z = sph(Ylm2, Theta, Phi)
plt.rcParams['font.sans-serif']=['Simhei']
plt.rcParams['axes.unicode_minus']=False
ax = fig.add_subplot(3,2,4,projection = "3d")
ax.set_title("Y%d%dscipy特殊函数" % (1, m))
ax.plot_surface(X, Y, Z, cmap="rainbow")
1 = 4
m = 2
Y]m=[]
num=100
theta = np.linspace(0, np.pi, num)
phi = np.linspace(0, 2 * np.pi, num)
Theta, Phi = np.meshgrid(theta, phi)
Ylm1 = Ball1(1, m, Phi, Theta)
for i in range(0, num):
    for j in range(0, num):
        Ylm1[i][j]=complex(Ylm1[i,j])
Ylm2 = np.abs(Ylm1)**2
X, Y, Z = sph(Ylm2, Theta, Phi)
plt.rcParams['font.sans-serif']=['Simhei']
plt.rcParams['axes.unicode_minus']=False
fig = plt.figure(figsize=(16,16))
ax = fig.add_subplot(3,2,5,projection = "3d")
ax.set_title("Y%d%d自己编写的特殊函数" % (1, m))
ax.plot_surface(X, Y, Z, cmap="rainbow")
1 = 4
m = 2
Y1m=[]
num=100
theta = np.linspace(0, np.pi, num)
phi = np.linspace(0, 2 * np.pi, num)
Theta, Phi = np.meshgrid(theta, phi)
Ylm = special.sph_harm(m, 1, Phi, Theta)
Ylm2 = np.abs(Ylm)**2
```

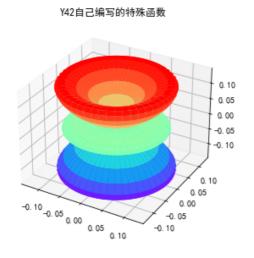
```
X, Y, Z = sph(Ylm2, Theta, Phi)
plt.rcParams['font.sans-serif']=['Simhei']
plt.rcParams['axes.unicode_minus']=False
ax = fig.add_subplot(3,2,6,projection = "3d")
ax.set_title("Y%d%dscipy特殊函数" % (1, m))
ax.plot_surface(X, Y, Z, cmap="rainbow")
plt.show()
```

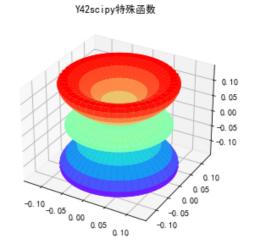












小结:几乎一模一样,但对于某些值,自己编的代码可能不能正常使用sympy求解

```
import numpy as np
import matplotlib.pyplot as plt
import scipy.special as spe
import scipy.constants as const
def sp(x, y, z):
    r = np.sqrt(x**2+y**2 +z**2)
    theta = np.arccos(z/r)
    phi = np.arctan(y/x)
    return np.array([r, theta, phi])
def wave(r, theta, phi, n, 1, m):
    return Rou(r, n, 1) * Ball1(l,m, phi, theta)
def wave_true(r, theta, phi, n, 1, m):
    return Rou(r, n, 1) * special.sph_harm(m, 1, phi, theta)
def width(n, 1):
   if 1 < n // 2:
        a = -1e-10 * (n + 1)
    else:
        a = -1e-10 * n**2
    return a, -a
n = 2
1 = 1
m = 0
a, b = width(n, 1)
x = np.linspace(a, b, 1000)
y = 0
z = np.linspace(a, b, 1000)
X, Z = np.meshgrid(x, z)
r, theta, phi = sp(X, y, Z)
psi = wave(r, theta, phi, n, 1, m)
density = np.abs(psi)**2
fig = plt.figure(dpi = 81)
ax = fig.gca()
ax.axis('auto')
ax.imshow(density,cmap='jet')
ax.set_title("空间密度分布self(n={},l={},m={})".format(n,l,m))
plt.show()
n = 3
1 = 1
m = 0
a, b = width(n, 1)
x = np.linspace(a, b, 1000)
y = 0
z = np.linspace(a, b, 1000)
X, Z = np.meshgrid(x, z)
r, theta, phi = sp(X, y, Z)
psi = wave(r, theta, phi, n, 1, m)
density = np.abs(psi)**2
fig = plt.figure(dpi = 81)
ax = fig.gca()
```

```
ax.axis('auto')
ax.imshow(density,cmap='jet')
ax.set\_title("空间密度分布self(n={},l={}),m={})" .format (n,1,m))
plt.show()
n = 5
1 = 2
m = 0
a, b = width(n, 1)
x = np.linspace(a, b, 1000)
y = 0
z = np.linspace(a, b, 1000)
X, Z = np.meshgrid(x, z)
r, theta, phi = sp(X, y, Z)
psi = wave(r, theta, phi, n, 1, m)
density = np.abs(psi)**2
fig = plt.figure(dpi = 81)
ax = fig.gca()
ax.axis('auto')
ax.imshow(density,cmap='jet')
ax.set_title("空间密度分布self (n={},l={},m={}) " .format (n,l,m))
plt.show()
n = 2
1 = 1
m = 0
a, b = width(n, 1)
x = np.linspace(a, b, 1000)
y = 0
z = np.linspace(a, b, 1000)
X, Z = np.meshgrid(x, z)
r, theta, phi = sp(X, y, Z)
psi = wave_true(r, theta, phi, n, 1, m)
density = np.abs(psi)**2
fig = plt.figure(dpi = 81)
ax = fig.gca()
ax.axis('auto')
ax.imshow(density,cmap='jet')
ax.set_title("空间密度分布scipy(n={},l={},m={})".format(n,l,m))
plt.show()
n = 3
1 = 1
m = 0
a, b = width(n, 1)
x = np.linspace(a, b, 1000)
y = 0
z = np.linspace(a, b, 1000)
X, Z = np.meshgrid(x, z)
r, theta, phi = sp(X, y, Z)
```

```
psi = wave_true(r, theta, phi, n, 1, m)
density = np.abs(psi)**2
fig = plt.figure(dpi = 81)
ax = fig.gca()
ax.axis('auto')
ax.imshow(density,cmap='jet')
ax.set_title("空间密度分布scipy(n={},l={},m={})" .format (n,1,m))
plt.show()
n = 5
1 = 2
m = 0
a, b = width(n, 1)
x = np.linspace(a, b, 1000)
y = 0
z = np.linspace(a, b, 1000)
X, Z = np.meshgrid(x, z)
r, theta, phi = sp(X, y, Z)
psi = wave_true(r, theta, phi, n, 1, m)
density = np.abs(psi)**2
fig = plt.figure(dpi = 81)
ax = fig.gca()
ax.axis('auto')
ax.imshow(density,cmap='jet')
ax.set_title("空间密度分布scipy(n={},l={},m={})".format(n,l,m))
plt.show()
```

