Funciones Radiales del Hidrógeno

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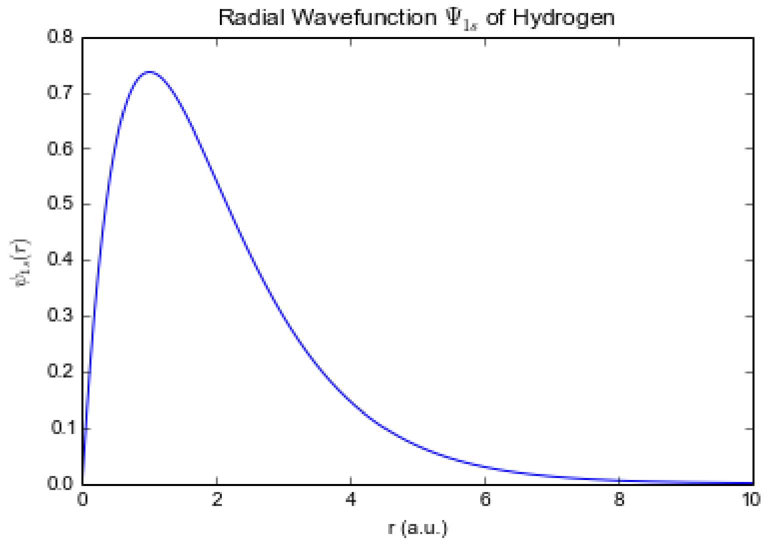
In [1]:
```
import numpy as np
import sympy as sp
import matplotlib.pyplot as plt

# Cosas útiles para utilizar luego
from sympy import oo
from __future__ import division

# Estética
sp.init_printing()
%matplotlib inline

#Definimos los simbolos que vamos a usar.

r=sp.Symbol('r',positive=True)
l=sp.Symbol('l',positive=True,integer=True)
n=sp.Symbol('n',positive=True,integer=True)
z=sp.Symbol('z',positive=True,integer=True)
k=sp.Symbol('k',positive=True)
```

In [2]:
```
# Función Radial Hidrogénica (con hipergeométricas)

def R_hyp(n,l,z,r):
    rho=2*r*z/n
    rnum = (2*z/n)**3 * sp.factorial(n+l)
    rden = (sp.factorial(2*l+1))**2 * 2*n * sp.factorial(n-l-1)
    rnorm = sp.sqrt(rnum/rden)
    rfunc = (rho)**l * sp.exp(-rho/2) * sp.hyper((-n+l+1,),(2*l+2,),
(rho))
    R = rnorm * rfunc
    return R
```

In [3]:
```
# Definición de los vectores para plotear

nsize=500
xmax=10.0
xmin=0.
x = np.linspace(xmin,xmax,nsize)
psi = np.zeros(nsize)
```

In [4]:
```
# Copiamos el array simbólico a numérico

for i in range(nsize):
  psi[i]=R_hyp(1,0,1,x[i])
```

In [5]:
```
# Ploteo

plt.plot(x,x*psi);
plt.title("Radial Wavefunction $\Psi_{1s}$ of Hydrogen");
plt.xlabel("r (a.u.)");
plt.ylabel("$\psi_{1s}(r)$");
```



In [6]:
```
# Integral simbólica

sp.integrate( (r * R_hyp(1,0,1,r))**2, (r,0,oo))
```

Out[6]: 1.0*hyper((0,), (2,), 0)**2

In [7]:
```
sp.integrate( (r * R_hyp(1,0,1,r))**2, (r,0,oo)).evalf()
```

Out[7]: 1.00000000000000

Ejercicios:

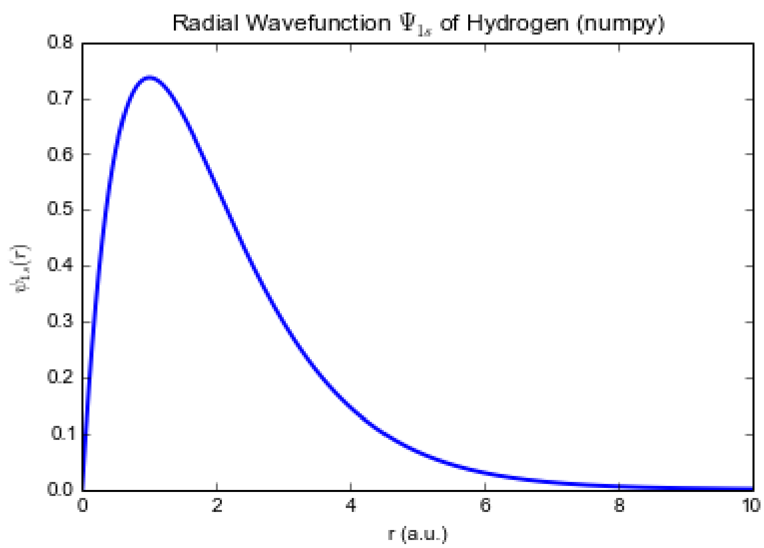
- Generar otras funciones de onda
- Chequear ortonormalidad
- Calcular los valores medio $\langle r \rangle$, $\langle r^2 \rangle$, $\langle \frac{1}{r} \rangle$

In [8]:
```
# Otra forma de hacerlo (con numpy)
```

In [30]:
```
from scipy import integrate
from scipy.special import hyp1f1
from math import factorial
```

In [31]:
```
def R1F1(n,l,z,r):
    rho=2*r*z/n
    rnum = (2*z/n)**3 * factorial(n+l)
    rden = (factorial(2*l+1))**2 * 2*n * factorial(n-l-1)
    rnorm = np.sqrt(rnum/rden)
    rfunc = (rho)**l * np.exp(-rho/2) * hyp1f1(-n+l+1,2*l+2,rho)
    R = rnorm * rfunc
    return R
```

In [32]:
```
r = np.linspace(0,10,200);
plt.plot(r,r*R1F1(1,0,1,r),'-',label='R1F1',linewidth=2);
plt.title("Radial Wavefunction $\Psi_{1s}$ of Hydrogen (numpy)");
plt.xlabel("r (a.u.)");
plt.ylabel("$\psi_{1s}(r)$");
```



In [33]:
```
# Integral

rR2=lambda r:(R1F1(1,0,1,r) * r)**2
Integral=integrate.quad(rR2,0,float('inf'))
print(Integral)
```

```
(1.0000000000000002, 1.3633023322217214e-10)
```

In [ ]: