SolucionFuncionesHcont

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1 Estados del Continuo del Hidrógeno

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```
In [3]: import numpy as np
        import sympy as sp
        import matplotlib.pyplot as plt

        # Cosas útiles para utilizar luego
        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)
```

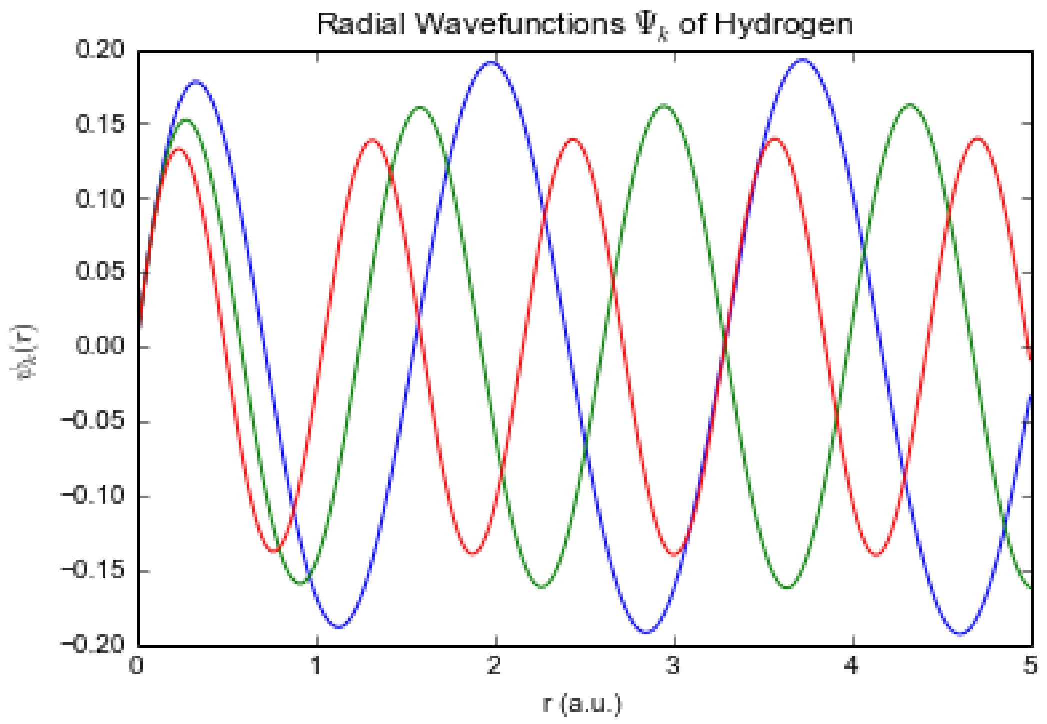
```
In [13]: # Función Radial Hidrogénica -- Estados del Contínuo (con hipergeométricas)

         def R_analytic(k,l,z,r):

             a = z/k # Parámetro de Sommerfeld

             # Imaginarios
             nj = 1j*a
             rho=-2*k*1j*r

             rnum = (2*z/nj)**3 * sp.gamma(nj+l+1)
             rden = (sp.gamma(2*l+2))**2 * 2*nj * sp.gamma(nj-l)
             rnorm = sp.sqrt(rnum/rden)
             rfunc = (2*k*r)**l * sp.exp(1j*k*r) * sp.hyper((-nj+l+1,),(2*l+2,),(rho))
             R = rfunc
             return R
```

```
In [113]:  # Definición de los vectores para plotear

           nsize=500
           xmax=5.0
           xmin=0.
```

```
        x = np.linspace(xmin,xmax,nsize)
        psi = np.zeros(nsize,dtype=complex)
        psi1 = np.zeros(nsize,dtype=complex)
        psi2 = np.zeros(nsize,dtype=complex)
```

```
In [114]: # Copiamos el array simbólico a numérico

        for i in range(nsize):
            psi[i]= R_analytic(3.5,0,1,x[i]).evalf()
            psi1[i]= R_analytic(4.5,0,1,x[i]).evalf()
            psi2[i]= R_analytic(5.50,0,1,x[i]).evalf()
```

```
In [115]: # Ploteo
        plt.plot(x,x*psi);
        plt.plot(x,x*psi1);
        plt.plot(x,x*psi2);
        plt.title("Radial Wavefunctions $\Psi_{k}$ of Hydrogen");
        plt.xlabel("r (a.u.)");
        plt.ylabel("$\psi_{k}(r)$");
```



2 Hydrogen Atom using Finite Differences

```
In [116]: from numpy import identity

        def Laplacian(x):
            h = x[1]-x[0] # assume uniformly spaced points
            n = len(x)
```

```
    M = -2*identity(n,'d')
    for i in range(1,n):
        M[i,i-1] = M[i-1,i] = 1
    return M/h**2
```

In [162]:
```
# Normalización de las funciones

from numpy import sqrt

def Normalizate(U,x):
    h = x[1]-x[0] # assume uniformly spaced points
    n = len(x)
    for j in range(0,n):
        suma = 0.0
        for i in range(1,n):
            suma = suma + U[i,j]**2
    suma = suma*h
    rnorm = 1/sqrt(suma)

    # Normalization
    rsign = 1
    if U[1,j] < 0:
        rsign = -1
    rnorm = rnorm * rsign
    for i in range(0,n):
        U[i,j] = U[i,j]*rnorm

    return U
```

In [163]:
```
# Generación de Hamiltoniano y diagonalización
```

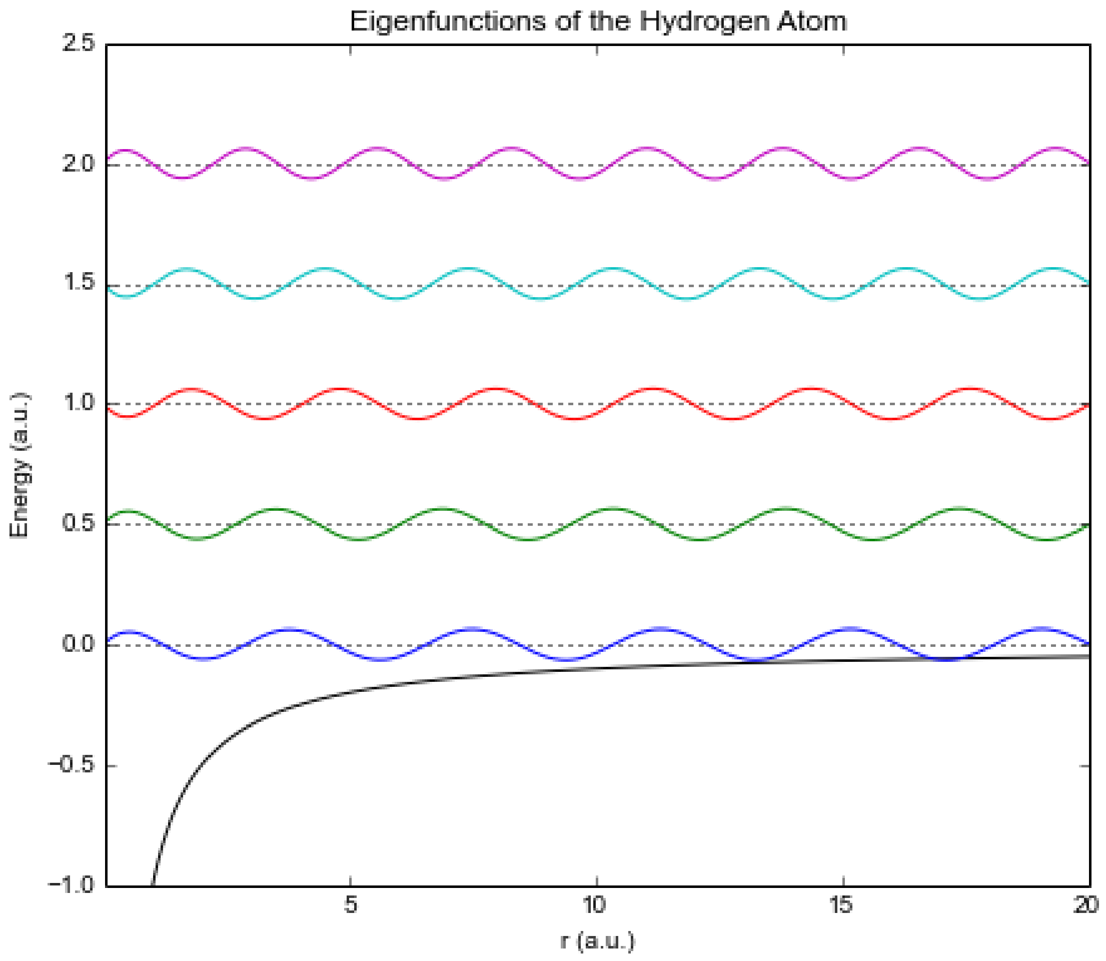
In [164]:
```
from numpy import diag, linspace, array
from numpy.linalg import eigh
from matplotlib.pyplot import axhline, xlabel, ylabel, plot, axis, figure, title, show

nfunctions = 5

# array definitions
nsize = 500
xmax=20.0
Dx = (xmax)/nsize
xmin=Dx
x = linspace(xmin,xmax,nsize)
T = array([nsize,nsize])
V = array([nsize,nsize])
H = array([nsize,nsize])
E = array([nsize])

# Kinetic (T) and  Potential (V)
T = (-0.5)*Laplacian(x)
V = -1/x

# Hamiltonian
H = T + diag(V)
```

```
         # Eigenvalues (E) and Eigenvectors (U)
         E,U = eigh(H)

         # Normalization
         U=Normalizate(U,x)
```

```
In [165]: # Plot
```

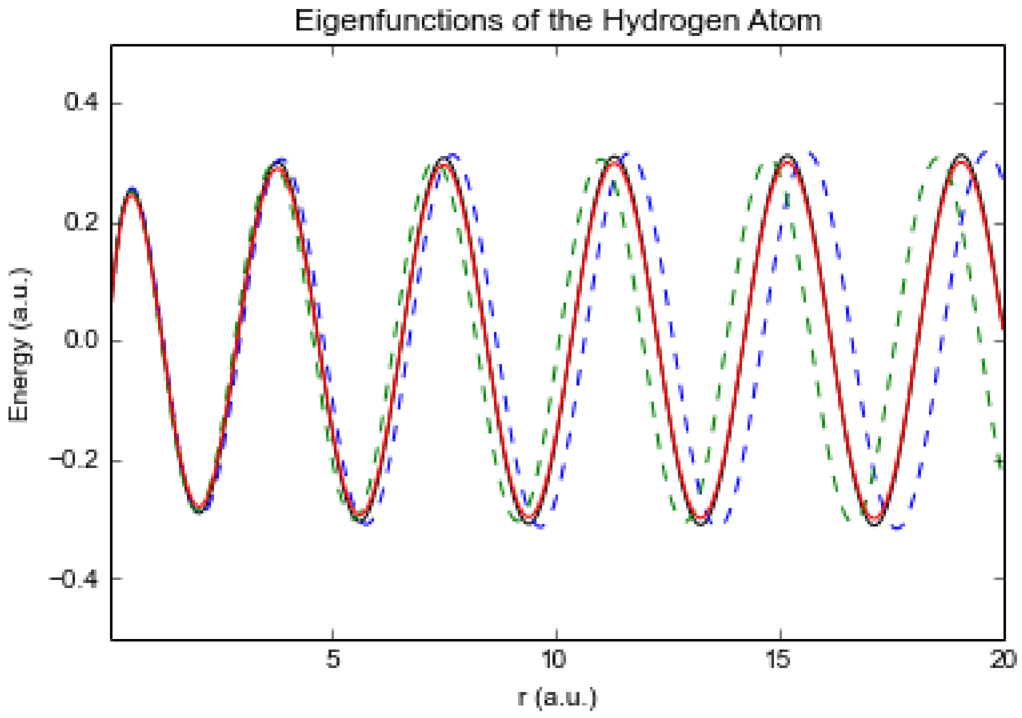
```
In [166]: #define plot size in inches (width, height) & resolution(DPI)
          fig = figure(figsize=(7, 6), dpi=100)

          # Plot the potential
          plot(x,V,color='k')

          # Plot wavefunctions
          ebase=-0.5
          for i in range(10,10+nfunctions):
              ebase=ebase+0.5
              # For each of the first few solutions, plot the energy level:
              axhline(y=ebase,color='k',ls=":")
              # as well as the eigenfunction, displaced the function
              # so they don't all pile up on each other:
              plot(x,U[:,i]+ebase)
              print("E=:",E[i])

          axis([xmin,xmax,-1,2.5])
          title("Eigenfunctions of the Hydrogen Atom")
          xlabel("r (a.u.)")
          ylabel("Energy (a.u.)")
          show()
```

```
('E=:', 1.2461512142646147)
('E=:', 1.5240081088389501)
('E=:', 1.8267764400253035)
('E=:', 2.1543750900184766)
('E=:', 2.5067383895924236)
```



3 Comparación entre Continuo Analítico y Diagonalizado

```
In [167]: #Ejemplo n=10
          n=10;
          nmed = 25

          yascale = abs(R_analytic(sqrt(2*E[n]),0,1,x[nmed]).evalf() / U[nmed,n]) ;
          yscale = float(yascale)

          # Copiamos el array simbólico a numérico
          # Le damos k=sqrt(2*E)
          for i in range(nsize):
              psi[i]= R_analytic(sqrt(2*E[n]),0,1,x[i]).evalf()
              psi1[i]= R_analytic(sqrt(2*E[n])-0.05,0,1,x[i]).evalf()
              psi2[i]= R_analytic(sqrt(2*E[n])+0.05,0,1,x[i]).evalf()

          plot(x,x*psi,color='k');
          plot(x,x*psi1,color='b',ls="--");
          plot(x,x*psi2,color='g',ls="--");
          plot(x,U[:,n]*yscale,color='r');

          axis([xmin,xmax,-0.5,0.5]);
          title("Eigenfunctions of the Hydrogen Atom")
          xlabel("r (a.u.)")
          ylabel("Energy (a.u.)")
          show()
```



```
In [ ]:
```