GUIA 1

Facundo L. Sanchez

In [1]:
```
import numpy as np
from scipy.special import hyp1f1
from scipy import integrate
from scipy.sparse import spdiags
from scipy.sparse.linalg import eigs
from numpy.linalg import eigh
import matplotlib.pyplot as plt
import time as tm
from math import factorial

from __future__ import division

%matplotlib inline
```

Defino la funcion de onda radial

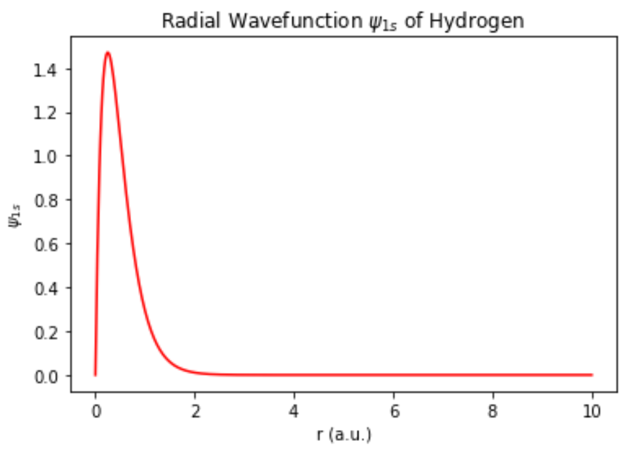
In [2]:
```
def R1F1(n,l,z,r):
    rho = 2 * r * z / n
    rnum = (2 * z / n)**3 * factorial(n + l)
    rden = (factorial(2*l+1))**2 * 2*n * factorial(n-l-1)
    rnorm = np.sqrt(rnum/rden)
    rfunc = (rho)**l * np.exp(-rho/2) * hyp1f1(-n+l+1, 2*l+2, rho)
    R = rnorm * rfunc
    return R
```

Defino los vectores para el plot

In [3]:
```
nlen = 500
rmax = 10.0
rmin = 0.0
r = np.linspace(rmin,rmax,nlen)
```

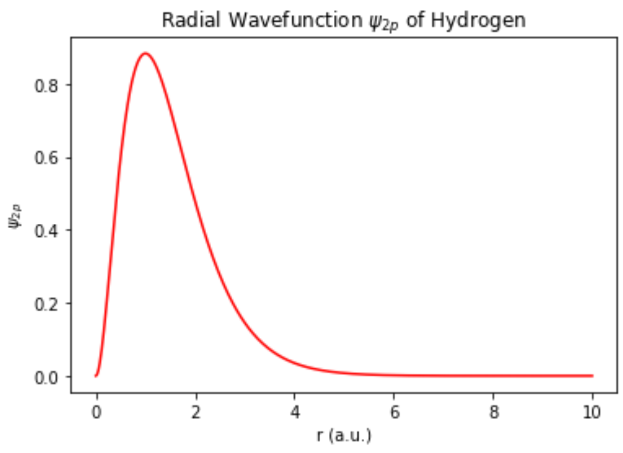
Plot para n = 1, l = 0, Z = 4

```
In [4]: psi_1 = R1F1(1,0,4,r)
        plt.plot(r, r*psi_1,'r')
        plt.title("Radial Wavefunction $\psi_{1s}$ of Hydrogen")
        plt.xlabel("r (a.u.)")
        plt.ylabel("$\psi_{1s}$")
        plt.show()
```



Plot para n = 2, l = 1, Z = 4

```
In [5]: psi_2 = R1F1(2,1,4,r)
        plt.plot(r, r*psi_2,'r')
        plt.title("Radial Wavefunction $\psi_{2p}$ of Hydrogen")
        plt.xlabel("r (a.u.)")
        plt.ylabel("$\psi_{2p}$")
        plt.show()
```



Chequeo ortonormalidad

```
In [6]: integrate.quad(lambda r:(r**2*R1F1(2,1,4,r)*R1F1(1,0,4,r)), 0, float('in
        f'))

Out[6]: (0.48384982573494933, 1.3072126370537772e-08)
```

- La parte radial no es ortogonal porque estoy en distintos niveles de energia

```
In [7]: integrate.quad(lambda r:(r**2*R1F1(2,1,4,r)**2), 0, float('inf'))
Out[7]: (0.9999999999999999, 1.3877796942138986e-08)

In [8]: integrate.quad(lambda r:(r**2*R1F1(1,0,4,r)**2), 0, float('inf'))
Out[8]: (1.0, 1.2956640677365438e-08)
```

- Las funciones estan normalizadas

Calculo $< r^k >, k = [-3, 3]$ ^ $k \neq 0$

```
In [9]: rMean_1s = []
        rMean_2p = []
        exponents_list = [exp for exp in range(-3,4) if exp is not 0]

        for i in exponents_list:
            rMean_2p.append(integrate.quad(lambda r:(r**(2+i)*R1F1(2,1,4,r)**2),
        0, float('inf')))
            rMean_1s.append(integrate.quad(lambda r:(r**(2+i)*R1F1(1,0,4,r)**2),
        0, float('inf')))

        print "Termino 1: 1s (n = 1, l = 0, Z = 4)"
        for i,exp in enumerate(exponents_list):
            print "< r^({:d}) > = {:.4f}; error = {:.2e}".format(exp,rMean_1s[i]
        [0],rMean_1s[i][1])

        print "\nTermino 2: 2p (n = 2, l = 1, Z = 4)"
        for i,exp in enumerate(exponents_list):
            print "< r^({:d}) > = {:.4f}; error = {:.2e}".format(exp,rMean_2p[i]
        [0],rMean_2p[i][1])
```

```
Termino 1: 1s (n = 1, l = 0, Z = 4)
< r^(-3) > = 8988.6307; error = 1.60e+03
< r^(-2) > = 32.0000; error = 9.02e-10
< r^(-1) > = 4.0000; error = 1.76e-09
< r^(1) > = 0.3750; error = 8.38e-09
< r^(2) > = 0.1875; error = 3.69e-09
< r^(3) > = 0.1172; error = 8.27e-10

Termino 2: 2p (n = 2, l = 1, Z = 4)
< r^(-3) > = 2.6667; error = 2.45e-11
< r^(-2) > = 1.3333; error = 1.26e-09
< r^(-1) > = 1.0000; error = 5.38e-10
< r^(1) > = 1.2500; error = 1.52e-08
< r^(2) > = 1.8750; error = 8.38e-10
< r^(3) > = 3.2812; error = 5.31e-09

/home/fakux/.local/lib/python2.7/site-packages/scipy/integrate/quadpack.p
y:364: IntegrationWarning: Extremely bad integrand behavior occurs at som
e points of the
  integration interval.
  warnings.warn(msg, IntegrationWarning)
```

- Se puede ver que el $< r^{-3} >_{1s}$ explota. Esto es asi porque el $l = 0$ neutraliza el termino de ρ^l ~ r^l de la R_{nl}

Kato

```
In [10]: from scipy.misc import derivative
```

Para el termino con $l = 0$

```
In [11]: derivative(lambda r: R1F1(1,0,4,r), 0, dx = 1e-10) / R1F1(1,0,4,0)

Out[11]: -4.000000330961484
```

Para el termino con $l = 1$

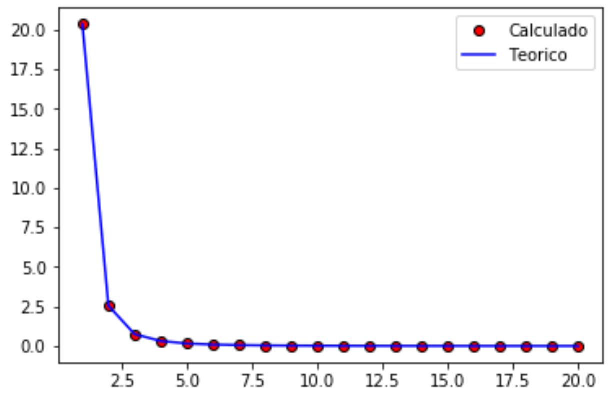
```
In [12]: print derivative(lambda r: R1F1(2,1,4,r), 0, dx = 1e-10) / R1F1(2,1,4,0)

inf

/home/fakux/.local/lib/python2.7/site-packages/ipykernel_launcher.py:1: R
untimeWarning: divide by zero encountered in double_scalars
  """Entry point for launching an IPython kernel.
```

- La funcion con $l = 1$ se anula en el origen, por eso no cumple Kato

Openheimmer

```
In [13]: from scipy.special import sph_harm as Yml
```

```
In [14]: ns = np.arange(1,21)
         y = np.zeros(len(ns))
         Z = 4

         for i,n in enumerate(ns):
             y[i] = np.abs(R1F1(n,0,Z,0)*Yml(0,0,0,0))**2

         plt.plot(ns,y,'ro',mec='k',label = 'Calculado')
         plt.plot(ns,(Z/ns)**3/np.pi,'b',label = 'Teorico')
         plt.legend(loc = 'best')
         plt.show()
```



- Obtuve lo esperado por Openheimmer

Virial

In [15]:
```
ur = lambda r: R1F1(1,0,Z,r)*r
Tfunc = lambda r: -0.5*derivative(ur, r, dx=1e-5, n=2)*ur(r)
Vfunc = lambda r: -Z/r*ur(r)**2
```

In [16]:
```
T = integrate.quad(Tfunc,0,np.inf)
V = integrate.quad(Vfunc,0,np.inf)
E_1 = T[0]+V[0]
print "Energia =",T[0]+V[0]
print "<V>/<T> =",V[0]/T[0]
```

```
Energia = -7.99999997699
<V>/<T> = -1.99999999425
```

In [17]:
```
l = 1
ur = lambda r: R1F1(2,l,Z,r)*r
Tfunc = lambda r: (-0.5*derivative(ur, r, dx=1e-5, n=2))*ur(r)+l*(l+1)/(
2*r**2)*ur(r)**2
Vfunc = lambda r: (-Z/r)*ur(r)**2
```

In [66]:
```
T = integrate.quad(Tfunc,0,np.inf)
V = integrate.quad(Vfunc,0,np.inf)
E_2 = T[0]+V[0]
print "Energia =",T[0]+V[0]
print "<V>/<T> =",V[0]/T[0]
```

```
Energia = -1.99999986978
<V>/<T> = -1.99999986978
```

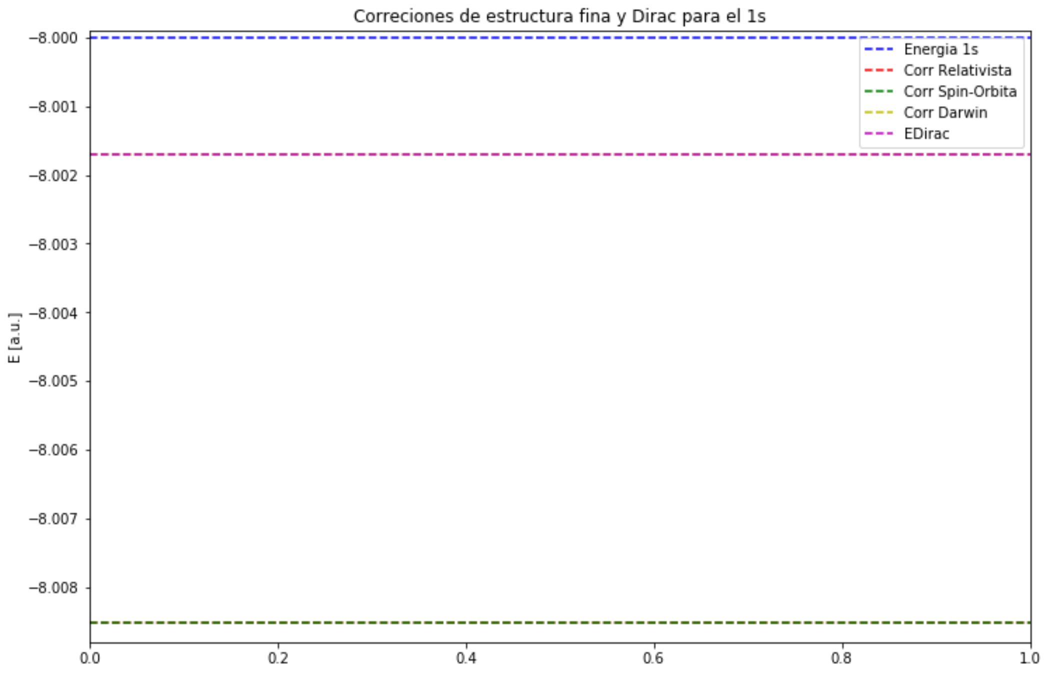
Correcciones de estructura fina

In [19]:
```
Z = 4
E1s = -Z**2/2
E2p = -Z**2/8
alpha = 1/137

# Correccion relativista (pag 198 del BJ)
deltaE_rel_1s = -alpha**2/2*(E1s**2 + 2*Z*E1s*rMean_1s[2][0] + Z**2*rMea
n_1s[1][0])
deltaE_rel_2p = -alpha**2/2*(E2p**2 + 2*Z*E2p*rMean_2p[2][0] + Z**2*rMea
n_2p[1][0])

# Correccion Spin-Orbita (pag 199 del BJ)
deltaE_SO_1s = 0 # pues l = 0 -> correccion SO nula
deltaE_SO_2p = alpha**2 * Z/4 * rMean_2p[0][0] * (3/2*(3/2+1) - 1*(1+1)
- 3/4)

# Correccion de Darwin (pag 200-201 del BJ)
deltaE_Darwin_1s = np.pi*alpha**2* Z/2 * np.abs((R1F1(1,0,Z,0)*Yml(0,0,0
,0)))**2
deltaE_Darwin_2p = np.pi*alpha**2* Z/2 * np.abs((R1F1(2,1,Z,0)*Yml(0,0,0
,0)))**2
# deltaE_Darwin_2p = 0, pues si l != 0 la funcion radial es nula en el o
rigen

# Energia Dirac
EDirac = lambda n,j,Z: 137**2*((1+(Z/137/(n-j-0.5+((j+0.5)**2-(Z/137)**2
)**0.5))**2)**(-0.5)-1)

EDirac1s = EDirac(1,0.5,4)
EDirac2p = EDirac(2,1.5,4)
```

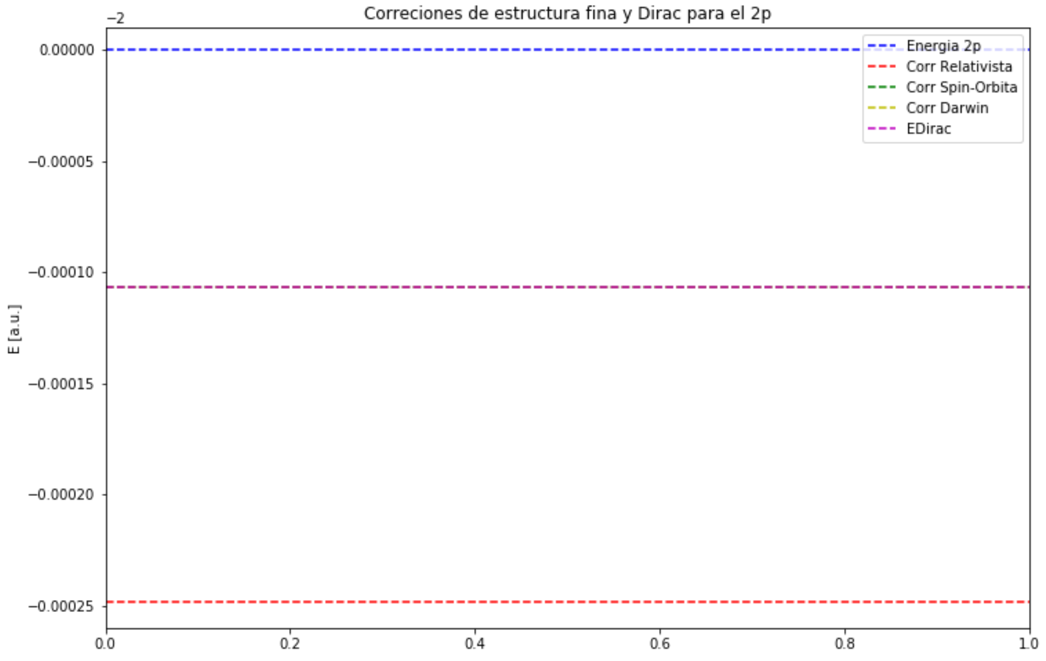
```
In [20]: Es = [E1s]
         Es.append(Es[-1] + deltaE_rel_1s)
         Es.append(Es[-1] + deltaE_SO_1s)
         Es.append(Es[-1] + deltaE_Darwin_1s)
         Es.append(EDirac1s)
         Es = np.array(Es)
         colors = list("brgym")
         print Es
         labs = ["Energia 1s", "Corr Relativista", "Corr Spin-Orbita", "Corr Darw
         in", "EDirac"]
         plt.figure(figsize=(12,8))
         for i in range(len(Es)):
             plt.axhline(Es[i],linestyle = 'dashed' ,label = labs[i], color = col
         ors[i])
         plt.ylim((-8.0088,-7.9999))
         plt.title("Correciones de estructura fina y Dirac para el 1s")
         plt.ylabel("E [a.u.]")
         plt.legend(loc='best')
```

```
[-8.         -8.00852469 -8.00852469 -8.00170494 -8.00170567]
```

```
Out[20]: <matplotlib.legend.Legend at 0x7f8db38f1750>
```



```
In [21]: Es = [E2p]
         Es.append(Es[-1] + deltaE_rel_2p)
         Es.append(Es[-1] + deltaE_SO_2p)
         Es.append(Es[-1] + deltaE_Darwin_2p)
         Es.append(EDirac2p)
         Es = np.array(Es)
         colors = list("brgym")
         print Es
         labs = ["Energia 2p", "Corr Relativista", "Corr Spin-Orbita", "Corr Darw
         in", "EDirac"]
         plt.figure(figsize=(12,8))
         for i in range(len(Es)):
             plt.axhline(Es[i], linestyle = 'dashed' ,label = labs[i], color = co
         lors[i])
         plt.ylim((-2.00026,-1.99999))
         plt.title("Correciones de estructura fina y Dirac para el 2p")
         plt.ylabel("E [a.u.]")
         plt.legend(loc='best')

         [-2.         -2.00024864 -2.00010656 -2.00010656 -2.00010657]

Out[21]: <matplotlib.legend.Legend at 0x7f8db39358d0>
```



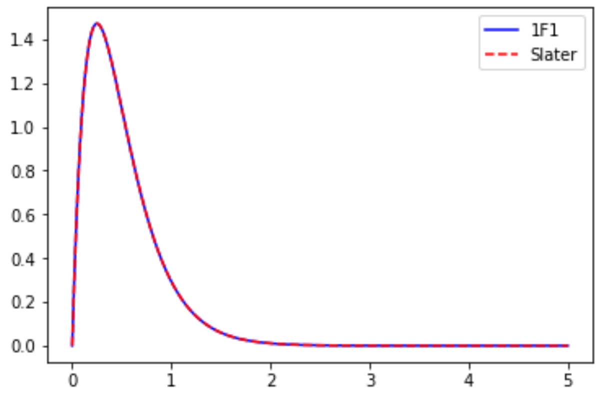
Funcion de onda en otras bases

Slater con coeficientes analiticos

In [22]:
```
def Slater_base(N,ksi,r):
    return (2*ksi)**(N+0.5)*r**(N-1)*np.exp(-ksi*r)/np.sqrt(factorial(2*
N))

def Slater_coeff(n,M,l):
    anum = (-1)**(M-1-l)*np.sqrt(factorial(n-l-1)*(factorial(n+l))*facto
rial(2*M))
    aden = np.sqrt(2*n)*factorial(M-l-1)*factorial(n-M)*factorial(M+l)
    return anum/aden

def Rnl_Slater(n,l,Z,r):
    R = 0
    for M in range(l+1,n+1):
        R = R + Slater_coeff(n,M,l)*Slater_base(M,Z/n,r)
    return R
```

In [23]:
```
r = np.linspace(0,5,1000)
plt.plot(r, r*R1F1(1,0,4,r), 'b', label="1F1")
plt.plot(r, r*Rnl_Slater(1,0,4,r), 'r--', label='Slater')
plt.legend(loc='best')
```

Out[23]:
```
<matplotlib.legend.Legend at 0x7f8de05e2a10>
```



Expansion en Slaters

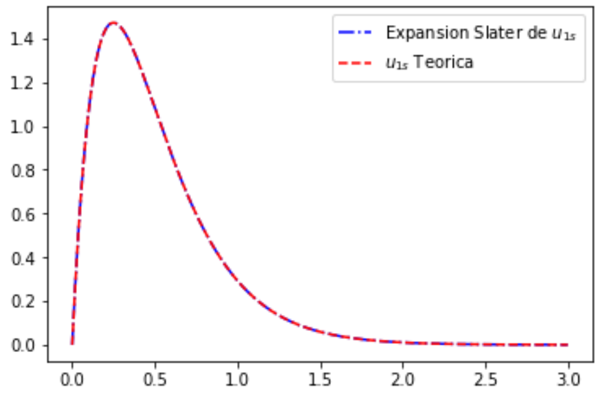
In [24]:
```
def Sij_Slater(i,j,alpha):
    return integrate.quad(lambda r: Slater_base(i+1,alpha,r)*Slater_base
(j+1,alpha,r),0,np.inf)[0]

def Overlap_Slater(N_Slat,alpha):
    M_overlap = np.zeros((N_Slat,N_Slat))
    for i in range(N_Slat):
        for j in range(i,N_Slat):
            S = Sij_Slater(i,j,alpha)
            M_overlap[i,j] = S
            M_overlap[j,i] = S
    return M_overlap

# Devuelve los coeficientes de la expansion en Slaters
def Slater_Expansion(n,l,Z,N_Slat):
    S = Overlap_Slater(N_Slat, Z/n)
    B = np.array([integrate.quad(lambda r: R1F1(n,l,Z,r)*Slater_base(i+1
,Z/n,r),0,np.inf)[0] for i in range(N_Slat)])
    return np.linalg.solve(S,B)
```

Expansion del 1s

```
In [25]: n = 1
         l = 0
         Z = 4
         # Cantidad de terminos de la base de Slater a usar
         N_Slat = 3

         Ci = Slater_Expansion(n,l,Z,N_Slat)
         Ci

Out[25]: array([1., 0., 0.])
```

```
In [26]: r = np.linspace(0,3,1000)
         wave1s = 0
         for i in range(N_Slat):
             wave1s = wave1s + Ci[i]*Slater_base(i+1,Z/n,r)
```

```
In [27]: plt.plot(r,r*wave1s,'b-.',label = 'Expansion Slater de $u_{1s}$')
         plt.plot(r,r*R1F1(n,l,Z,r), 'r--' ,label = '$u_{1s}$ Teorica')
         plt.legend(loc='best')
         plt.show()
```

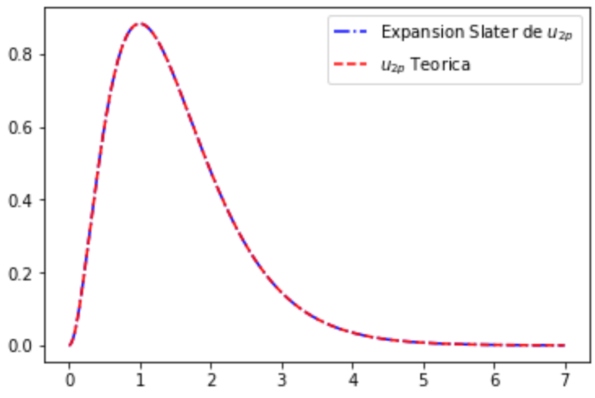


Expansion del 2p

```
In [28]: n = 2
         l = 1
         Z = 4
         # Cantidad de terminos de la base de Slater a usar
         N_Slat = 3

         Ci = Slater_Expansion(n,l,Z,N_Slat)
         Ci

Out[28]: array([2.22044605e-16, 1.00000000e+00, 6.24500451e-16])
```

```
In [29]: r = np.linspace(0,7,1000)
         wave2p = 0
         for i in range(N_Slat):
             wave2p = wave2p + Ci[i]*Slater_base(i+1,Z/n,r)
```

In [30]:
```
plt.plot(r,r*wave2p,'b-.',label = 'Expansion Slater de $u_{2p}$')
plt.plot(r,r*R1F1(n,l,Z,r), 'r--' ,label = '$u_{2p}$ Teorica')
plt.legend(loc='best')
plt.show()
```



Expansion en Laguerre

In [31]:
```
from scipy.special import eval_genlaguerre
```

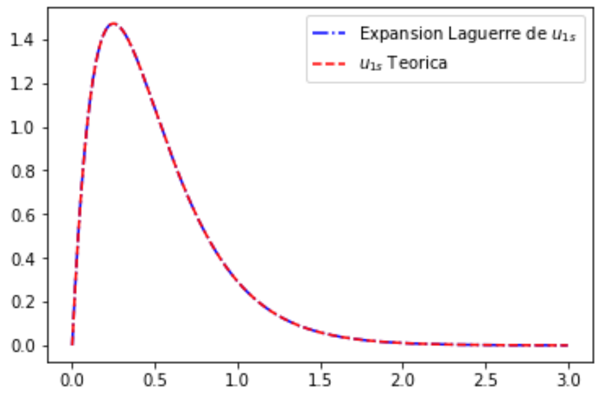
In [32]:
```
def Laguerre_Base(n,l,Z,r):
    rho = 2*r*Z/n
    return (rho)**l*np.exp(-rho/2)*eval_genlaguerre(n-l-1,2*l+1,rho)

def Laguerre_Expansion(n,l,Z):
    num = integrate.quad(lambda r: R1F1(n,l,Z,r)*Laguerre_Base(n,l,Z,r),
0,np.inf)[0]
    den = integrate.quad(lambda r: Laguerre_Base(n,l,Z,r)**2,0,np.inf)[0
]
    return num/den
```

Expansion 1s

In [33]:
```
n = 1
l = 0
Z = 4

# Como los Laguere asociados son base ortogonal, solo calculo el coefici
ente, que es la normalizacion
C = Laguerre_Expansion(n,l,Z)
```

In [34]:
```
r = np.linspace(0,3,1000)
wave1s = C*Laguerre_Base(n,l,Z,r)
```

In [35]:
```
plt.plot(r,r*wave1s,'b-.',label = 'Expansion Laguerre de $u_{1s}$')
plt.plot(r,r*R1F1(n,l,Z,r), 'r--' ,label = '$u_{1s}$ Teorica')
plt.legend(loc='best')
plt.show()
```

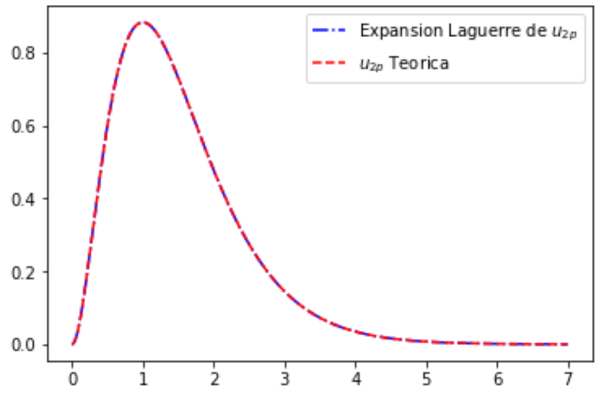


Expansion 2p

In [36]:
```
n = 2
l = 1
Z = 4

C = Laguerre_Expansion(n,l,Z)
```

In [37]:
```
r = np.linspace(0,7,1000)
wave2p = C*Laguerre_Base(n,l,Z,r)
```

In [38]:
```
plt.plot(r,r*wave2p,'b-.',label = 'Expansion Laguerre de $u_{2p}$')
plt.plot(r,r*R1F1(n,l,Z,r), 'r--' ,label = '$u_{2p}$ Teorica')
plt.legend(loc='best')
plt.show()
```



Soluciones Numericas

Diferencias finitas (Diagonalizacion)

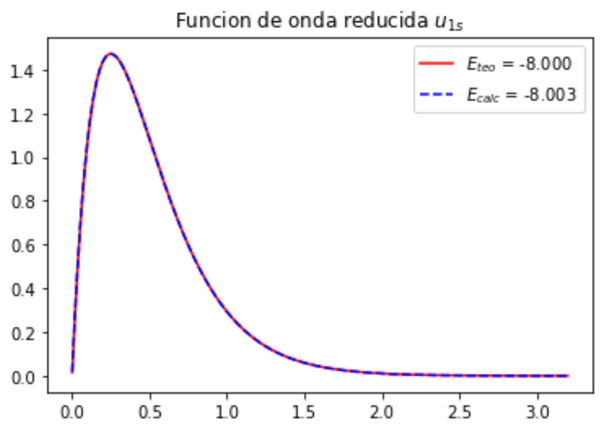
```
In [39]: # usando numpy
         def H_matriz(ri,rf,N,Z,l):
             r = np.linspace(ri,rf,N)
             h = (rf-ri)/float(N)

             offDiag_der2 = np.ones(len(r)-1)
             diag_cent = l*(l+1)/(2*r**2)
             T_matriz = (np.diag(offDiag_der2,-1) - 2*np.eye(N,dtype=float) + np.
         diag(offDiag_der2,1))/(-2*h**2) \
                         + np.diag(diag_cent)

             diag_V = -Z/r
             V_matriz = np.diag(diag_V)

             return T_matriz+V_matriz, r
```

Solucion para el 1s (n = 1, l = 0, Z = 4)

```
In [40]: Z = 4
         rmin = 0.001
         rmax = 3.2
         npuntos = 3000
         l = 0
         H, r = H_matriz(rmin,rmax,npuntos,Z,l)
```

```
In [41]: # E son las energias, v las respectivas funciones de onda
         # sin normalizar como columnas de una matriz v de autovectores
         E, v = eigh(H)
         E[np.where(E<0)]

Out[41]: array([-8.00315295, -1.96523371])
```

```
In [42]: j = 0 # indice que maneja la el autovector a usar
         n = 1 # numero cuantico ppal
         sgn = -1 # manejo el signo porque a veces dan al reves las cosas

         # normalizo las funciones de onda al intervalo que uso
         w1s_teo = r*R1F1(n,l,Z,r)/np.sqrt(np.trapz((r*R1F1(n,l,Z,r))**2,r))
         w1s_calc = v[:,j]/np.sqrt(np.trapz(v[:,j]**2,r))*sgn
         # plotteo
         plt.plot(r,w1s_teo,'r',label = '$E_{teo}$'+' = {:.3f}'.format(-Z**2/(2*n
         **2)))
         plt.plot(r,w1s_calc,'b--',label = '$E_{calc}$'+' = {:.3f}'.format(E[j]))
         plt.title("Funcion de onda reducida $u_{1s}$")
         plt.legend(loc='best')

Out[42]: <matplotlib.legend.Legend at 0x7f8db3602710>
```



Solucion para el 2p (n = 2, l = 1, Z = 4)

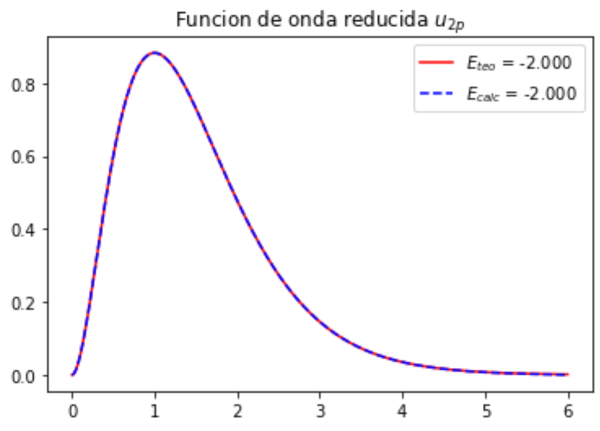
In [43]:
```
Z = 4
rmin = 0.001
rmax = 6
npuntos = 3000
l = 1
H, r = H_matriz(rmin,rmax,npuntos,Z,l)
```

In [44]:
```
# E son las energias, v las respectivas funciones de onda
# sin normalizar como columnas de una matriz v de autovectores
E, v = eigh(H)
E[np.where(E<0)]
```

Out[44]:
```
array([-1.99955468, -0.87345039, -0.21225942])
```

In [45]:
```
j = 0 # indice que maneja la el autovector a usar
n = 2 # numero cuantico ppal
sgn = -1 # manejo el signo porque a veces dan al reves las cosas

# normalizo las funciones de onda al intervalo que uso
w1s_teo = r*R1F1(n,l,Z,r)/np.sqrt(np.trapz((r*R1F1(n,l,Z,r))**2,r))
w1s_calc = v[:,j]/np.sqrt(np.trapz(v[:,j]**2,r))*sgn
# plotteo
plt.plot(r,w1s_teo,'r',label = '$E_{teo}$'+' = {:.3f}'.format(-Z**2/(2*n
**2)))
plt.plot(r,w1s_calc,'b--',label = '$E_{calc}$'+' = {:.3f}'.format(E[j]))
plt.title("Funcion de onda reducida $u_{2p}$")
plt.legend(loc='best')
```

Out[45]:
```
<matplotlib.legend.Legend at 0x7f8daf071a50>
```



Variacional con 4 gaussianos

In [46]:
```
from scipy.linalg import eigh
```

```
In [47]: def Overlap_ij(alpha,i,j):
             Sij = ( np.pi / (alpha[i] + alpha[j]) )**(1.5)
             return Sij

         def Matriz_Overlap(alpha):
             nsize = len(alpha)
             S = np.zeros((nsize,nsize))
             for i in range(0,nsize):
                 for j in range(i,nsize):
                     S[i,j]=Overlap_ij(alpha,i,j)
                     S[j,i]=S[i,j]
             return S
```

```
In [48]: # Elemento de matriz de cinetica
         def Tij(alpha,l,i,j):
             rnum = 3 * np.pi**(1.5) * alpha[i] * alpha[j]
             rden =  (alpha[i] + alpha[j] )**(2.5)
             Tij = rnum/rden + l*(l+1)/2*np.pi**0.5/(2*(alpha[i]+alpha[j])**0.5)
             return Tij


         # Elemento de matriz de potencial
         def Vij(alpha,Z,i,j):
             Vij =  Z*( -2*np.pi )  /  (alpha[i] + alpha[j])
             return Vij

         # Matriz del Hamiltoniano en la base
         def Matriz_H(alpha,l,Z):
             nsize = len(alpha)
             H = np.zeros((nsize,nsize))
             for i in range(0,nsize):
                 for j in range(i,nsize):
                     H[i,j]=Tij(alpha,l,i,j) + Vij(alpha,Z,i,j)
                     H[j,i]=H[i,j]
             return H
```

1s Variacional

```
In [49]: # Defino los alphas que voy a usar para el exponente de los gaussianos
         alpha = np.array([13.00773, 1.962079, 0.444529, 0.1219492])

         Z = 4
         l = 0

         # Genero las matrices de overlap y Hamiltonianos
         H = Matriz_H(alpha,l,Z)
         S = Matriz_Overlap(alpha)
```

```
In [50]: E,C = eigh(H,S,type=1)
         E[np.where(E<0)]

Out[50]: array([-7.64993215, -1.94651165, -0.83248831])
```

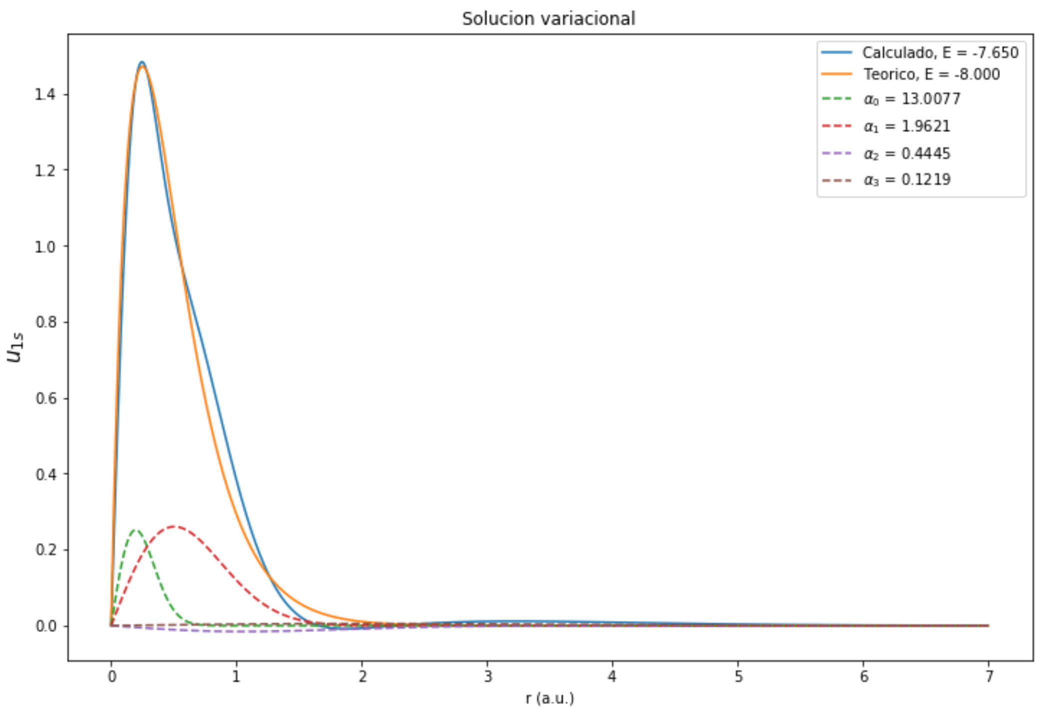
```
In [51]: def psi(Ci,Alpha,x):
             nsize = len(Ci)
             res = 0
             for i in range(0,nsize):
                 res = res + Ci[i]*np.exp(-Alpha[i]*x**2)
             return res
```

In [52]:
```
# array definitions
npts = 1000
xmin=0.0
xmax=7.0
x = np.linspace(xmin,xmax,npts)
wave1s = np.zeros(npts)
wave2p = np.zeros(npts)
```

In [53]:
```
# El autovector es la funcion de onda
C0 = C[:,0]
wave1s = psi(-C0,alpha,x)

# Normalizo
norm_cuad = np.trapz((wave1s*x)**2,x)
wave1s = wave1s/norm_cuad**0.5
```

In [54]:
```
plt.figure(figsize=(12,8))
plt.plot(x,x*wave1s, label = 'Calculado, E = {:.3f}'.format(E[0])); # No
rmalizo en ese intervalo
plt.plot(x,x*R1F1(1,l,Z,x),label = 'Teorico, E = {:.3f}'.format(-Z**2/(2
*1**2)))
plt.title("Solucion variacional");
plt.xlabel("r (a.u.)");
plt.ylabel("$u_{1s}$",size=15);
for i in range(len(alpha)):
    plt.plot(x,x*(-C0[i])*np.exp(-alpha[i]*x**2), label = r'$\alpha_{:d}
$ = {:.4f}'.format(i,alpha[i]), linestyle='dashed')
plt.legend(loc='best')
```

Out[54]:
```
<matplotlib.legend.Legend at 0x7f8db367ef10>
```



2p variacional

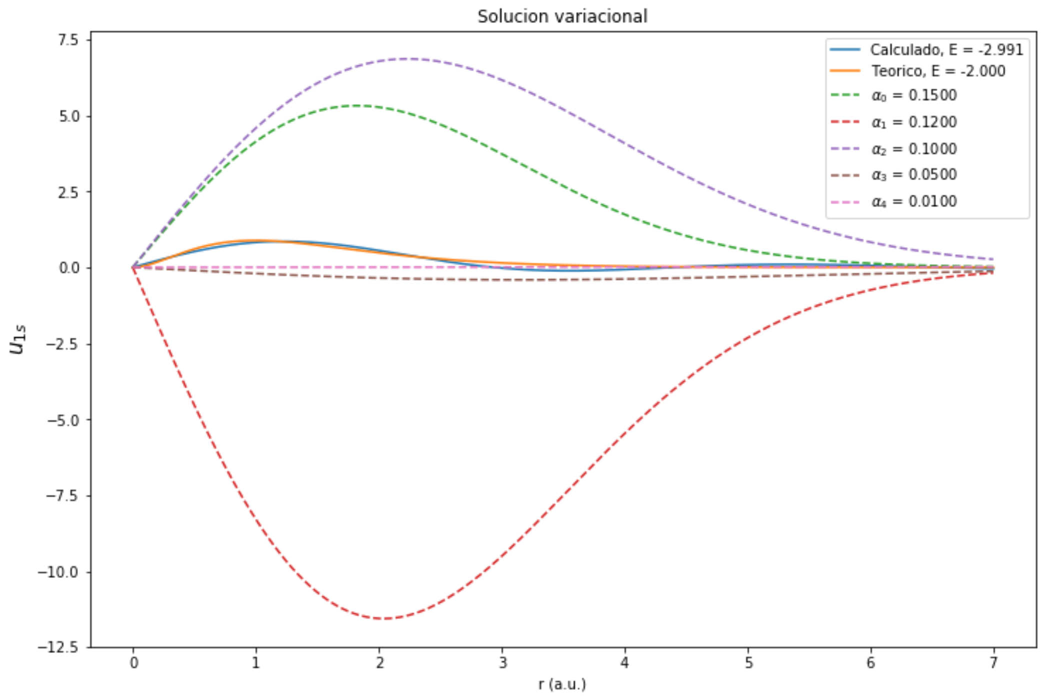
```
In [55]: # Defino los alphas que voy a usar para el exponente de los gaussianos
         alpha = np.array([0.15,0.12,0.1, 0.05, 0.01])

         Z = 4
         l = 1

         # Genero las matrices de overlap y Hamiltonianos
         H = Matriz_H(alpha,l,Z)
         S = Matriz_Overlap(alpha)
```

```
In [56]: E,C = eigh(H,S,type=1)
         E[np.where(E<0)]

Out[56]: array([-2.99058447, -1.02046294, -0.53375585, -0.33587597, -0.1923691 ])
```

```
In [57]: # array definitions
         npts = 1000
         xmin=0.0
         xmax=7.0
         x = np.linspace(xmin,xmax,npts)
         wave1s = np.zeros(npts)
         wave2p = np.zeros(npts)
```

```
In [58]: # El autovector es la funcion de onda
         C0 = C[:,0]
         wave1s = psi(-C0,alpha,x)

         # Normalizo
         norm_cuad = np.trapz((wave1s*x)**2,x)
         wave1s = wave1s/norm_cuad**0.5
```

```
In [59]: plt.figure(figsize=(12,8))
         plt.plot(x,x*wave1s, label = 'Calculado, E = {:.3f}'.format(E[0])); # No
         rmalizo en ese intervalo
         plt.plot(x,x*R1F1(2,l,Z,x),label = 'Teorico, E = {:.3f}'.format(-Z**2/(2
         *2**2)))
         plt.title("Solucion variacional");
         plt.xlabel("r (a.u.)");
         plt.ylabel("$u_{1s}$",size=15);
         for i in range(len(alpha)):
             plt.plot(x,x*(-C0[i])*np.exp(-alpha[i]*x**2), label = r'$\alpha_{:d}
         $ = {:.4f}'.format(i,alpha[i]), linestyle='dashed')
         plt.legend(loc='best')

Out[59]: <matplotlib.legend.Legend at 0x7f8db3713350>
```



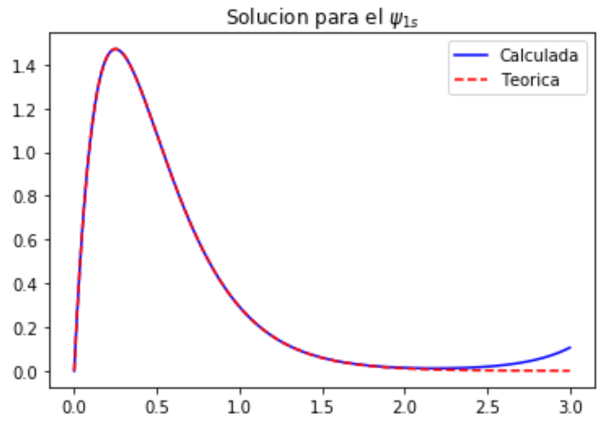
Solucion Numerica

Solucion para el 1s

```
In [60]: def g(y,x,E):
             l = 0
             Z = 4
             return [y[1],2*(-Z/x+l*(l+1)/(2*x**2)-E)*y[0]]
```

```
In [61]: # Valores iniciales de phi(x) y phi'(x)
         initialY = 0,0.01
         # Valor tentativo de E
         E = -8
         Z = 4
         l = 0
         x = np.linspace(1e-10,3,10000)
         # Solucion ecuación diferencial
         sol = integrate.odeint(g,initialY,x,(E,))
```

In [62]:
```
psi = sol[:,0]
psi = psi/np.trapz((psi)**2,x=x)**0.5
# Ploteo de solución
plt.plot(x, psi, color='b',label = 'Calculada')
w1s = x*R1F1(1,0,Z,x)
w1s = w1s/np.trapz(w1s**2,x=x)**0.5
plt.plot(x,w1s,'r--', label = 'Teorica')
plt.legend(loc='best')
plt.title("Solucion para el $\psi_{1s}$")
plt.show()
```

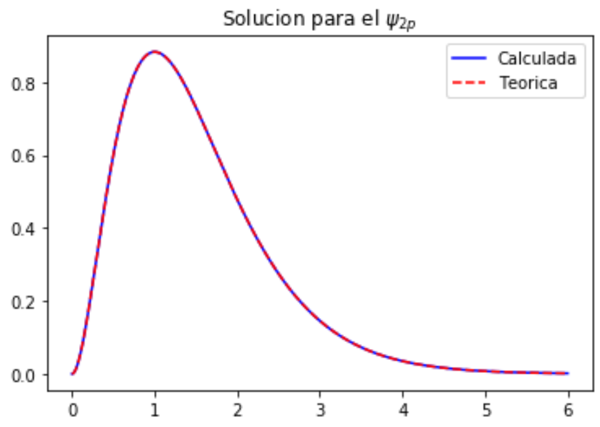


Solucion para el 2p

In [63]:
```
def g(y,x,E):
    l = 1
    Z = 4
    return [y[1],2*(-Z/x+l*(l+1)/(2*x**2)-E)*y[0]]
```

In [64]:
```
# Valores iniciales de phi(x) y phi'(x)
initialY = 0,0.0001
# Valor tentativo de E
E = -2
x = np.linspace(1e-5,6,10000)
# Solucion ecuación diferencial
sol = integrate.odeint(g,initialY,x,(E,))
```

```
In [65]: psi = sol[:,0]
         psi = psi/np.trapz((psi)**2,x=x)**0.5
         # Ploteo de solución
         plt.plot(x, psi, color='b',label = 'Calculada')
         w1s = x*R1F1(2,1,Z,x)
         w1s = w1s/np.trapz(w1s**2,x=x)**0.5
         plt.plot(x,w1s,'r--', label = 'Teorica')
         plt.legend(loc='best')
         plt.title("Solucion para el $\psi_{2p}$")
         plt.show()
```



```
In [ ]:
```