Hidrógeno Variacional

Cálculo Variacional del Estado Fundamental del Hidrógeno

In [1]:
```
from numpy import    linspace, zeros, array,pi
from scipy.linalg import      eigh ,eigvalsh

%matplotlib inline
from matplotlib.pyplot importplot, title, legend, show, axhline,\
                                    xlabel, ylabel, axis, figure
```

In [2]:
```
nsize =4
S= zeros((nsize,nsize))
H= zeros((nsize,nsize))
Alpha =zeros((nsize))
Ci =zeros((nsize))
```

In [3]:
```
# Datos Iniciales para variacional
Alpha[0] = 13.00773
Alpha[1] = 1.962079
Alpha[2] = 0.444529
Alpha[3] = 0.1219492
```

In [4]:
```
#Cálculo de Overlaps      Sij=<xi|xj>

def overlap(Alpha,p,q):
    spq =( pi / (Alpha[p] + Alpha[q]) )**(3./2.)

    return spq

for i in range(0,nsize):
    for jin range(i,nsize):
        S[i,j]=overlap(Alpha,i,j)
        S[j,i]=S[i,j]
```

In [5]:
```
S
```

Out[5]:
```
array([[    4.19640644e-02,   9.61391815e-02,   1.12857904e-01,
            1.17042513e-01],
       [    9.61391815e-02,   7.16316708e-01,   1.49147774e+00,
            1.85084232e+00],
       [    1.12857904e-01,   1.49147774e+00, 6.64247101e+00,
            1.30602054e+01],
       [    1.17042513e-01,   1.85084232e+00, 1.30602054e+01,
            4.62286682e+01]])
```

In [6]:
```
#Cálculo de Hamiltoniano Hij=<xi| H |xj>


        #Cálculo de Energía Cinética     Tij=<xi|-1/2 D^2|xj>
        def Tkin(Alpha,p,q):
            rnum =3 *pi**(3./2.) *Alpha[p] *Alpha[q]
            rden=   (Alpha[p] + Alpha[q] )**(5./2.)
            Tpq =rnum/rden
            return Tpq


        #Cálculo de Energía Potencial     Vij=<xi|-Z/r |xj>
        def Vpot(Alpha,p,q):
            Vpq=   ( -2*pi)      /    (Alpha[p] + Alpha[q])
            return Vpq

        for i in range(0,nsize):
            for jin range(i,nsize):
                H[i,j]=Tkin(Alpha,i,j) + Vpot(Alpha,i,j)
                H[j,i]=H[i,j]
```

In [7]:
```
H
```

Out[7]:
```
array([[     0.57726847,   0.07200247, -0.3215405,    -0.43612626],
       [    0.07200247,   0.50704993, -0.98918483,  -2.37741992],
       [-0.3215405,      -0.98918483,  -2.63808243,  -7.34221693],
       [-0.43612626,    -2.37741992,  -7.34221693, -17.30516271]])
```

In [8]:
```
# Solución autovalores generalizados (H-ES)(C)=0
        #Sólo Autovalores!

        Ener = eigvalsh(H,S,type=1)
        Ener
```

Out[8]:
```
array([ -0.49927841,      0.11321392,   2.59229957,  21.14436519])
```

In [9]:
```
Ener[0]
```

Out[9]:
```
-0.49927840566748505
```

In [10]:
```
# Solución  autovalores generalizados (H-ES)(C)=0

Ener,coef =eigh(H,S,type=1)
Ci =coef[:,0]
```

In [11]:
```
def psi(Ci,Alpha,x):
    from math import  exp
    nsize =len(Ci)
    sum =0.0
    for iin range(0,nsize):
        sum =sum +Ci[i]*exp(-Alpha[i]*x**2)
return sum
```

In [12]:
```
# array definitions
npts =100
xmin=0.0
xmax=4.0
x = linspace(xmin,xmax,npts)
wave1s =zeros(npts)
```

In [13]:
```
for i in range(0,npts):
    wave1s[i] =psi(-Ci,Alpha,x[i])
```

In [14]:
```
plot(x,wave1s);
axis([xmin,xmax,0,0.6]);
title("Ground State Wavefunction ofHydrogen Atom (variational)");
xlabel("r (a.u.)");
ylabel("\\Psi_{1s}");
```