Numerov Hidro Final Artigo

May 2, 2022

[1]:
```
import matplotlib.pyplot as plt
import numpy as np
from numpy import random
from random import random
x = np.linspace(-10,10,1001)

def  V(x):
     L=0                            #secondary quantum number
     Vx=(L*(L+1))/(x*x)-2./x        #effective potential
     return  Vx

def vec_max(dim,x):                  #left maximum
    xmax=0
    N=dim
    for j in range(int(N)):
        if j<int(N) and abs(x[j])>xmax:
           xmax=abs(x[j])
        else:
           continue
    return xmax

def  nrovl(y0, y1, x0, E, h, iflag):   #left solution
     q0  =  (E-V(x0))
     q1  =  (E-V(x0+h))
     q2  =  (E-V(x0+h+h))
     p0  =  (1 + h*h*q0/12)
     p1   =   2*(1 - 5*h*h*q1/12)
     p2   =   1 + h*h*q2/12
     y2   =  (p1*y1-p0*y0)/p2
     if iflag<1:
        print(" x0 = ", x0," y0 = ", y0," V = ",V(x0))
        print(" x1 = ", x0+h," y1 = ",y1," V = ",V(x0+h)," y2 = ",y2)
     return  y2

def  nrovr(y0, y1, x0, E, h, iflag):   #right solution
     q0  =  (E-V(x0))
     q1  =  (E-V(x0-h))
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    q2  =  (E-V(x0-h-h))
    p0  =  (1 + h*h*q0/12)
    p1   =   2*(1 - 5*h*h*q1/12)
    p2   =   1 + h*h*q2/12
    y2   =  (p1*y1-p0*y0)/p2
    if iflag<1:
       print(" x_100 = ", x0," y0_100 = ", y0," V = ",V(x0))
       print(" x_99 = ", x0-h," y_99 = ",y1," V = ",V(x0-h)," y_98 = ",y2)
    return  y2

def espectro(xl,xu,h,delta,eps,dim,nmax,kmax,Ein,Vmax,dE,iflag):

    xx=list(range(dim));     yy=list(range(dim));
    yl=list(range(dim));     yr=list(range(dim))
    ee=list(range(nmax));    ff=list(range(nmax));    ff2=list(range(nmax))
    yy1=list(range(dim));    yy2=list(range(dim));    yy3=list(range(dim))
    nk=list(range(nmax))
    E_old = Ein;   E = Ein + dE


    # here yy1, yy2 and yy3 represent the three wave functions that the
    #code wants to find, if you want to find more solutions you must add
    #new parameters in the code

    for M in range(nmax):
       print("  ****************   Eigenvalue  #",M+1,"  ***************** ")

       f_old=0
       for k in range(kmax): #iteration for candidate eigenvalue

           imatch=0

           for j in range(dim-1):  #classical right turning point
               xx[0]=xl;          xx[dim-1]=xu
               DE1 = E - V(xx[j])
               xx[j+1] = xx[j]+h
               DE2 = E - V(xx[j+1])
               D1D2=DE1*DE2
               if D1D2<=0  and DE1 > 0:  #match point
                  imatch = j+1
                  print(" imatch = ",imatch," xmatch = %2.3f" %(xx[imatch]),"␣
↪V(xmatch) = %2.5f" %(V(xx[imatch])),"  E = %2.4f" %(E))

           xmatch=xx[imatch]
           ii=range(imatch+2)
           i_lim = ii[2:imatch+2]
```

```
            xx[0]=xl;  xx[1]=xl+h   #initial values
            yy[0]=0;   yy[1] = delta


            for i in i_lim:                                          #numerov left␣
↪solution
                yy[i]=nrovl(yy[i-2],yy[i-1],xx[i-2],E,h,iflag)
                xx[i]= xx[i-1]+h

            jjj=list(range(dim+1))
            j_lim = list(jjj[imatch-1:dim+1])
            comp_j=len(j_lim)
            jj=sorted(j_lim,key=abs,reverse=True)

            for i in range(dim):
                if i<=imatch+1:
                   yl[i]=yy[i]
                if i>imatch+1:
                   yl[i]=0

            for i in jj:                                             #numerov right␣
↪solution
                if i==dim:
                    yr[dim-1]=0
                if i==(dim-2):
                    yr[dim-2]=2*delta
                if i<(dim-2):
                    yr[i]=nrovr(yr[i+2],yr[i+1],xx[i+2],E,h,iflag)
                    xx[i]= xx[i+1]-h

            for i in range(imatch-1):
                yr[i]=0

            ymatch=yy[imatch]
            yrmatch=yr[imatch]
            ylmatch=yl[imatch]


            if ymatch != 0:
                scale=yrmatch/ymatch
            else:
                continue

            for t in range(imatch+1):    #  y_left
                yy[t] = yy[t]*scale
                yl[t] = -yl[t]*scale
            yl[imatch+1]=-yl[imatch+1]*scale
```

```
            ymatch=yy[imatch]
            dlmatch=yy[imatch+1]*scale-yy[imatch-1]                    # dif1_left

            t_lim=list(range(dim+1))
            tt=list(t_lim[imatch+1:dim])

            drmatch=yr[imatch+1]-yr[imatch-1]                          # dif1_right

            f =(dlmatch-drmatch)/(2*h)

            for t in tt:                        #  y_right
                yy[t] = yr[t]


            delta_E=-f*(E-E_old)/(f-f_old)

            if abs(delta_E)<eps:  # determination of the root (energy) of f(E)␣
↪by the secant method
                ee[M] = E
                nk[M] = k
                ff[M] = f
                k = kmax
                break
            else:
                f_old=f;  E_old=E;   E = E + 24*dE

        if M==0:
                   E = E + 126*dE
           for j in range(dim):
               yy1[j]=yy[j]
        if M==1:
           E = E + 3*dE
           for j in range(dim):
               yy2[j]=yy[j]
        if M==2:
           E = E_old + 6*dE
           for j in range(dim):
               yy3[j]=yy[j]

        print(" k = %2d   E_old = %2.3f    Eingen = %2.3f   f_old = %2.3e   f =␣
↪%2.3e   delta_E = %2.3e" %(nk[M],E_old,ee[M],f_old,f,delta_E))
        print()

    return ee, xx, yy1, yy2, yy3

#=============================================================================
```

```
a=0.001; b= 60.001; h=0.01
xl=a; xu=b; D = xu-xl
delta = 0.02; eps = 0.0001
dim=int(D/h); kmax=300; nmax=3
n =0; iflag=0
Rydberg=13.605693122994

x0=xl; y0=0. ; y1=delta; iflag=1
nrovl(y0,y1,x0,0,h,iflag)
nrovr(y0,y1,xu,0,h,iflag)

dE = delta/4
Ein = -1.6
Vmax= 0.

print("␣
 ↪==========================================================================")
print("  ")
print("         Potential : V(x) = (L*(L+1))/(x*x)-2./x    (Hydrogen L=0)   ")
print("  ")
print("␣
 ↪==========================================================================")

print(" E_in = %2.4f" %(Ein)," dE = ",dE," h = ",h," dim = ",dim)
print("  ")


ee,xx,yy1,yy2,yy3=espectro(xl,xu,h,delta,eps,dim,nmax,kmax,Ein,Vmax,dE,iflag)

A=1.                        # amplitude normalization in 1 unit
ymax1=vec_max(dim,yy1);   ymax2=vec_max(dim,yy2);   ymax3=vec_max(dim,yy3)

for i in range(dim):      # amplitude normalization
    yy1[i] = yy1[i]/ymax1;  yy2[i] = yy2[i]/ymax2;   yy3[i] = yy3[i]/ymax3

colors =['b','r','g','c','m','y','k'];    #color list (blue, red, green, cyan,␣
 ↪yellow, magenta and black)


plt.figure(figsize=(8, 6), dpi=800)
plt.plot(x,V(x),color=colors[6],linewidth=2)
plt.ylim(-10,1)
plt.xlim(a,10)
plt.xlabel('x')
plt.ylabel('Effective Potential')
plt.grid()
```

```
plt.show()


plt.figure(figsize=(8, 6), dpi=800)
plt.plot(xx,yy1,color=colors[0])
plt.plot(xx,yy2,'--',color=colors[1])
plt.plot(xx,yy3,':',color=colors[2])
plt.legend([' y1','  y2','  y3'],prop={"size":15},frameon=True)
plt.ylim(-0.7,1.1)
plt.xlim(0,40)
plt.xlabel('x')
plt.ylabel('Eigenfunctions (normalized amplitude)')
plt.grid()
plt.show()

efic=list(range(nmax));  I=list(range(nmax));   eI=list(range(nmax))

S=A*(xu-xl)                      # Born normalizatiom
l0=0; l1=0; l2=0
N=10000
for i in range(N):               # integral of y*y with the Monte Carlo method
    y = A*random()
    j=np.random.randint(dim)
    yj1=yy1[j]*yy1[j];   yj2=yy2[j]*yy2[j];   yj3=yy3[j]*yy3[j]
    if y <= yj1:
       l0 += 1
    if y <= yj2:
       l1 += 1
    if y <= yj3:
       l2 += 1

efic[0] = float(l0)/N;  efic[1] = float(l1)/N;  efic[2] = float(l2)/N
I[0] = S*efic[0];       I[1] = S*efic[1];       I[2] = S*efic[2]
eI[0] = (S/np.sqrt(N))*np.sqrt(efic[0]*(1-efic[0]))
eI[1] = (S/np.sqrt(N))*np.sqrt(efic[1]*(1-efic[1]))
eI[2] = (S/np.sqrt(N))*np.sqrt(efic[2]*(1-efic[2]))

print("  ")
print("  probability normalization ")
print(" efic1 = %2.3f   I1 = %2.3f   eI1 = %2.3f" %(efic[0],I[0],eI[0]))
print(" efic2 = %2.3f   I2 = %2.3f   eI2 = %2.3f" %(efic[1],I[1],eI[1]))
print(" efic2 = %2.3f   I2 = %2.3f   eI2 = %2.3f" %(efic[2],I[2],eI[2]))

for i in range(dim):                             # probability normalization
    yy1[i]=yy1[i]/np.sqrt(I[0]); yy2[i]=yy2[i]/np.sqrt(I[1]); yy3[i]=yy3[i]/np.
 ↪sqrt(I[2])
```

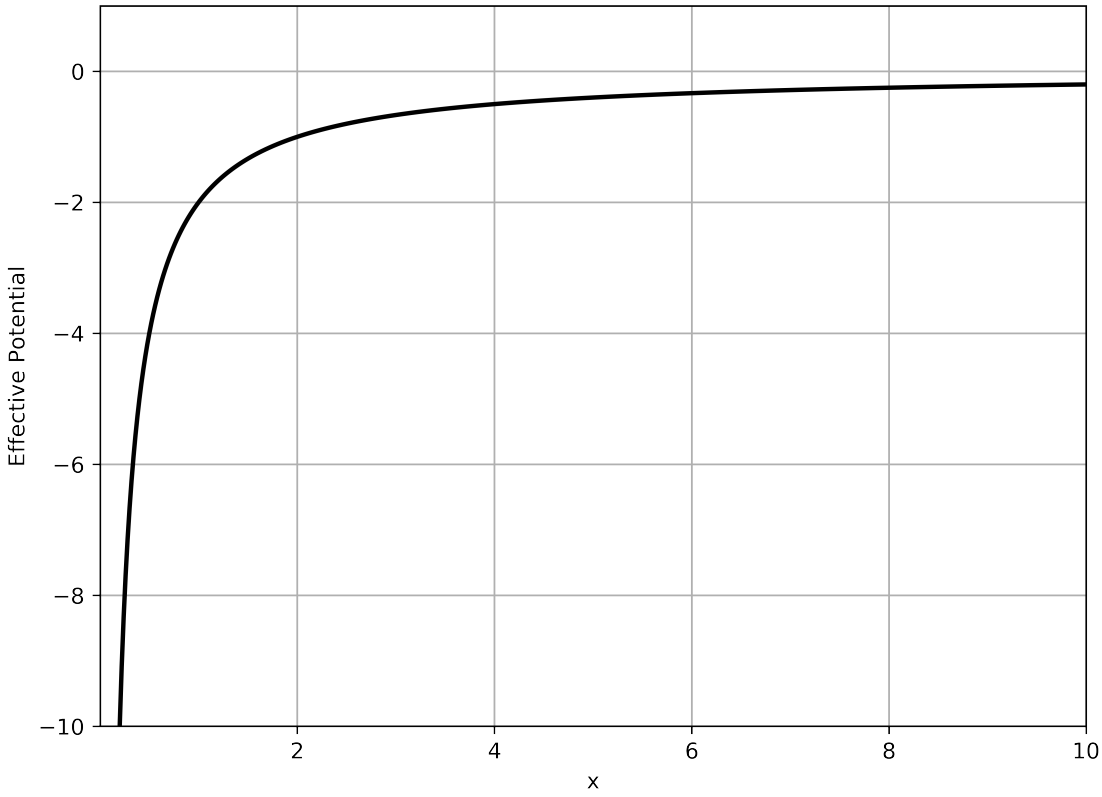
```
ymax1=vec_max(dim,yy1);   ymax2=vec_max(dim,yy2);   ymax3=vec_max(dim,yy3)

S0=ymax1*ymax1*(xu-xl);   S1=ymax2*ymax2*(xu-xl);   S2=ymax3*ymax3*(xu-xl)

l0=0;  l1=0; l2=0           # checking probability
N=10000
for i in range(N):
    y1 = ymax1*ymax1*random(); y2 = ymax2*ymax2*random(); y3 =␣
 ↪ymax3*ymax3*random()
    j=np.random.randint(dim)
    yj1=yy1[j]*yy1[j];   yj2=yy2[j]*yy2[j];    yj3=yy3[j]*yy3[j]
    if y1<= yj1:
       l0 += 1
    if y2 <= yj2:
       l1 += 1
    if y3 <= yj3:
       l2 += 1

efic[0] = float(l0)/N;  efic[1] = float(l1)/N;  efic[2] = float(l2)/N
I[0] = S0*efic[0];      I[1] = S1*efic[1];      I[2] = S2*efic[2]
eI[0] = (S0/np.sqrt(N))*np.sqrt(efic[0]*(1-efic[0]))
eI[1] = (S1/np.sqrt(N))*np.sqrt(efic[1]*(1-efic[1]))
eI[2] = (S2/np.sqrt(N))*np.sqrt(efic[2]*(1-efic[2]))

print("  ")
print("  checking probability ")
print(" efic1 = %2.3f   I1 = %2.3f   eI1 = %2.3f" %(efic[0],I[0],eI[0]))
print(" efic2 = %2.3f   I2 = %2.3f   eI2 = %2.3f" %(efic[1],I[1],eI[1]))
print(" efic3 = %2.3f   I3 = %2.3f   eI3 = %2.3f" %(efic[2],I[2],eI[2]))

et=[-1,-1/4,-1/9];      sig_e=[0.005,0.005,0.005]
print(" ")
print("  energy spectrum (E/Ry)  ",['{:2.3f}'.format(energia) for energia in␣
 ↪ee])
print("  uncertainty in energy (E/Ry) ",[' {:2.3f}'.format(sige) for sige in␣
 ↪sig_e])
print("  theoretical spectrum (E/Ry)     ",['{:2.3f}'.format(energia) for␣
 ↪energia in et])
print()




plt.figure(figsize=(8, 6), dpi=800)
plt.plot(xx,yy1,color=colors[0])
plt.plot(xx,yy2,'--',color=colors[1])
```

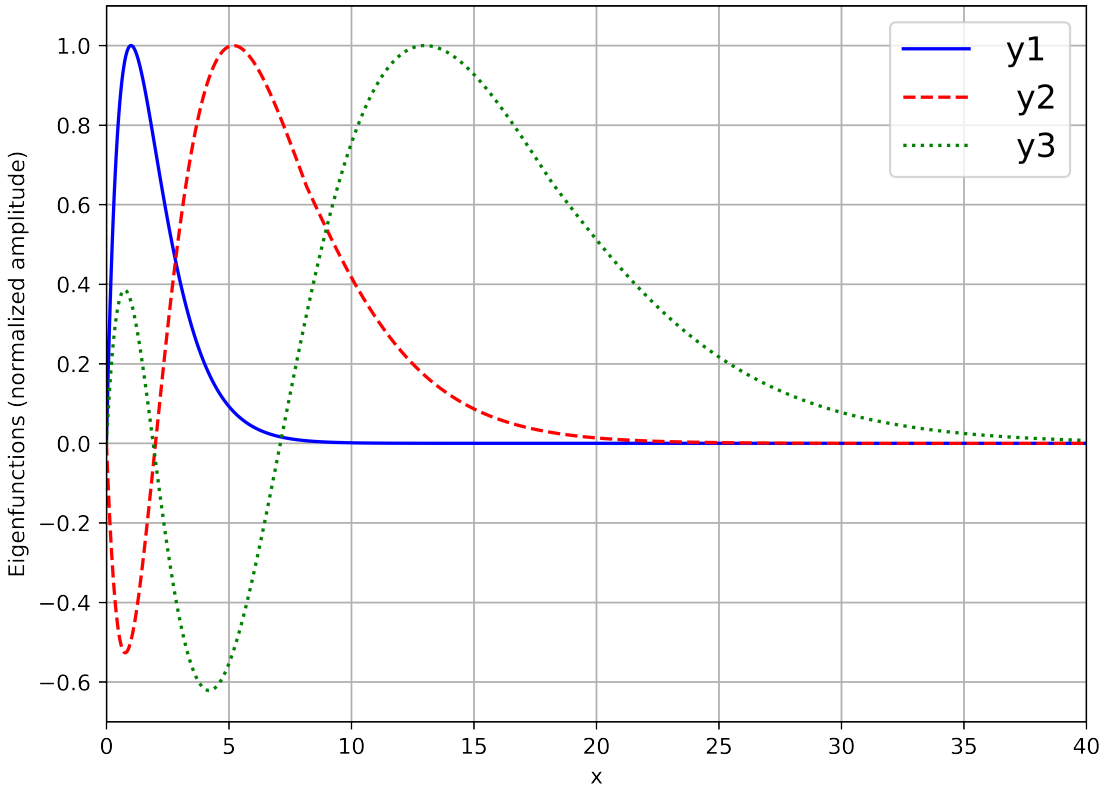
```
plt.plot(xx,yy3,':',color=colors[2])
plt.legend(['y1','y2','y3'],prop={"size":15},frameon=True)
plt.ylim(-0.3,0.8)
plt.xlim(0,40)
plt.xlabel('x')
plt.ylabel('Normalized Eigenfunctions')
plt.grid(True)
plt.show()


eev=list(range(nmax))
for j in range(nmax):
    eev[j]=Rydberg*ee[j]

sig_e=[Rydberg*0.005,Rydberg*0.005,Rydberg*0.005]
et=[-Rydberg,-0.25*Rydberg,-(1./9)*Rydberg]

print(" ")
print("  energy spectrum (eV)  ",['{:2.3f}'.format(energia) for energia in eev])
print("  uncertainty in energy (eV) ",[' {:2.3f}'.format(sige) for sige in␣
 ↪sig_e])
print("  espectro teorico (eV)     ",['{:2.3f}'.format(energia) for energia in␣
 ↪et])
print()

se = [0.005,0.005,0.005]
nx = [1,2,3]
N  = len(ee)
x  = list(range(N))
y  = list(range(N))
ey = list(range(N))

for i in range(N):
     y[i]   = np.log(-ee[i])
     x[i]   = np.log(nx[i])
     ey[i]  = -se[i]/ee[i]

isig2 = [1/(ey[0]*ey[0]),1/(ey[1]*ey[1]),1/(ey[2]*ey[2])]

sig2  = 1/sum(isig2)
w     = [sig2*isig2[0],sig2*isig2[1],sig2*isig2[2]]

x_M   = [w[0]*x[0],w[1]*x[1],w[2]*x[2]]
y_M   = [w[0]*y[0],w[1]*y[1],w[2]*y[2]]
xy_M  = [w[0]*x[0]*y[0],w[1]*x[1]*y[1],w[2]*x[2]*y[2]]

xM = sum(x_M);   yM = sum(y_M);    xyM = sum(xy_M)
```

```
x2_M  = [w[0]*(x[0])**2,w[1]*(x[1])**2,w[2]*(x[2])**2]
x2M  = sum(x2_M)
sx_2 = [w[0]*(x[0]-xM)**2,w[1]*(x[1]-xM)**2,w[2]*(x[2]-xM)**2]
sy_2 = [w[0]*(y[0]-yM)**2,w[1]*(y[1]-yM)**2,w[2]*(y[2]-yM)**2]
sx2  = sum(sx_2)
sy2  = sum(sy_2)
sxy = xyM - (xM*yM)


a = sxy/sx2;       b = yM - a*xM;       r = np.sqrt(sx2/sy2)*a

alfa = a;      beta = -np.exp(b)

siga = np.sqrt(sig2/sx2);     sigb = siga*np.sqrt(x2M);     e_beta = -sigb*beta

print("  ")
print("   a = %2.3f  ea = %2.3f    b = %2.3f  eb = %2.3f       r = %2.9f"␣
 ↪%(a,siga,b,sigb,-r),"     y = ax + b (y = log|En|, x=log(n))")
print("   alfa = %2.3f  e_alfa = %2.3f     beta = %2.3f  e_beta = %2.3f"␣
 ↪%(alfa,siga,beta,e_beta),"   En (calc) = %2.3f*n**(%2.3f)" %(beta,alfa)," En␣
 ↪(teor) = -1*n**(-2)  " )


x=np.linspace(1,12,100)
xx=list(range(8))
et=list(range(8));   eobs=list(range(8));   sig_e=list(range(8))

for i in range(8):
    et[i]   = -1/(i+1)**2
    eobs[i] = beta*(i+1)**alfa
    sig_e[i] = 0.005

plt.figure()
plt.figure(figsize=(8, 6), dpi=800)
plt.scatter(nx,ee,c="blue")
plt.plot(x,beta*x**alfa,'-',color=colors[1])
plt.xlabel('n')
plt.ylabel('Energy_n (E/Ry)')
plt.ylim(-1.1,0)
plt.legend(['  Adjust to energy levels '],prop={"size":15},frameon=False)
plt.grid(True)
plt.show()

print()
print("  theoretical spectrum   (E/Ry):",['{:2.3f}'.format(energia) for energia␣
 ↪in et])
```

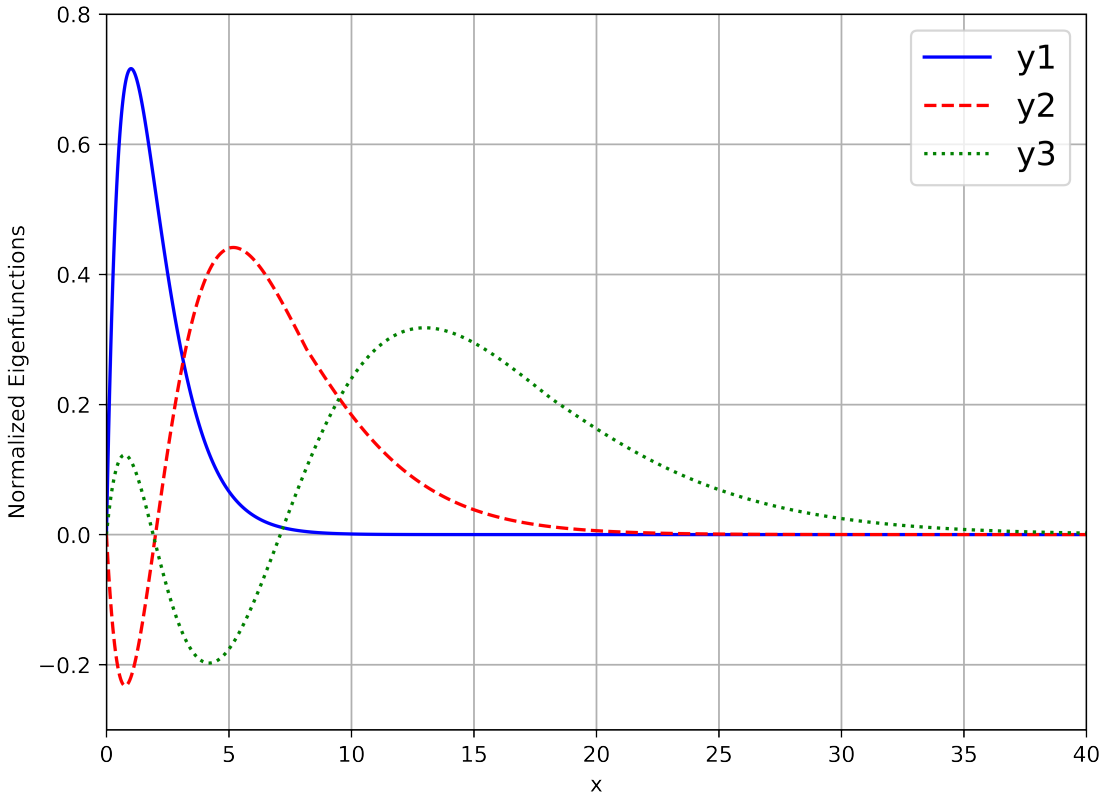
```
print("  predicted spectrum  (E/Ry):",['{:2.3f}'.format(energia) for energia in␣
 ↪eobs])
print(" predicted uncertainty (eE/Ry):",[' {:2.3f}'.format(energia) for energia␣
 ↪in sig_e])
```

```
 ========================================================================

         Potential : V(x) = (L*(L+1))/(x*x)-2./x    (Hydrogen L=0)

 ========================================================================
 E_in = -1.6000  dE =  0.005  h =  0.01  dim =  6000

  ****************   Eigenvalue  # 1   *****************
 imatch =  126  xmatch = 1.261  V(xmatch) = -1.58604  E = -1.5950
 imatch =  136  xmatch = 1.361  V(xmatch) = -1.46951  E = -1.4750
 imatch =  148  xmatch = 1.481  V(xmatch) = -1.35044  E = -1.3550
 imatch =  162  xmatch = 1.621  V(xmatch) = -1.23381  E = -1.2350
 imatch =  180  xmatch = 1.801  V(xmatch) = -1.11049  E = -1.1150
 imatch =  201  xmatch = 2.011  V(xmatch) = -0.99453  E = -0.9950
 k =  5   E_old = -1.115    Eingen = -0.995   f_old = 1.052e+25   f = -3.124e+21
delta_E = -3.560e-05

  ****************   Eigenvalue  # 2   *****************
 imatch =  548  xmatch = 5.481  V(xmatch) = -0.36490  E = -0.3650
 imatch =  817  xmatch = 8.171  V(xmatch) = -0.24477  E = -0.2450
 k =  1   E_old = -0.365    Eingen = -0.245   f_old = 5.129e+12   f = -4.319e+08
delta_E = -1.011e-05

  ****************   Eigenvalue  # 3   *****************
 imatch =  870  xmatch = 8.701  V(xmatch) = -0.22986  E = -0.2300
 imatch =  1819  xmatch = 18.191  V(xmatch) = -0.10994  E = -0.1100
 k =  1   E_old = -0.230    Eingen = -0.110   f_old = -1.184e+09   f =
-2.755e+03   delta_E = 2.792e-07


C:\Users\felip\anaconda3\lib\site-packages\ipykernel_launcher.py:9:
RuntimeWarning: invalid value encountered in true_divide
  if __name__ == '__main__':
C:\Users\felip\anaconda3\lib\site-packages\ipykernel_launcher.py:9:
RuntimeWarning: divide by zero encountered in true_divide
  if __name__ == '__main__':
```

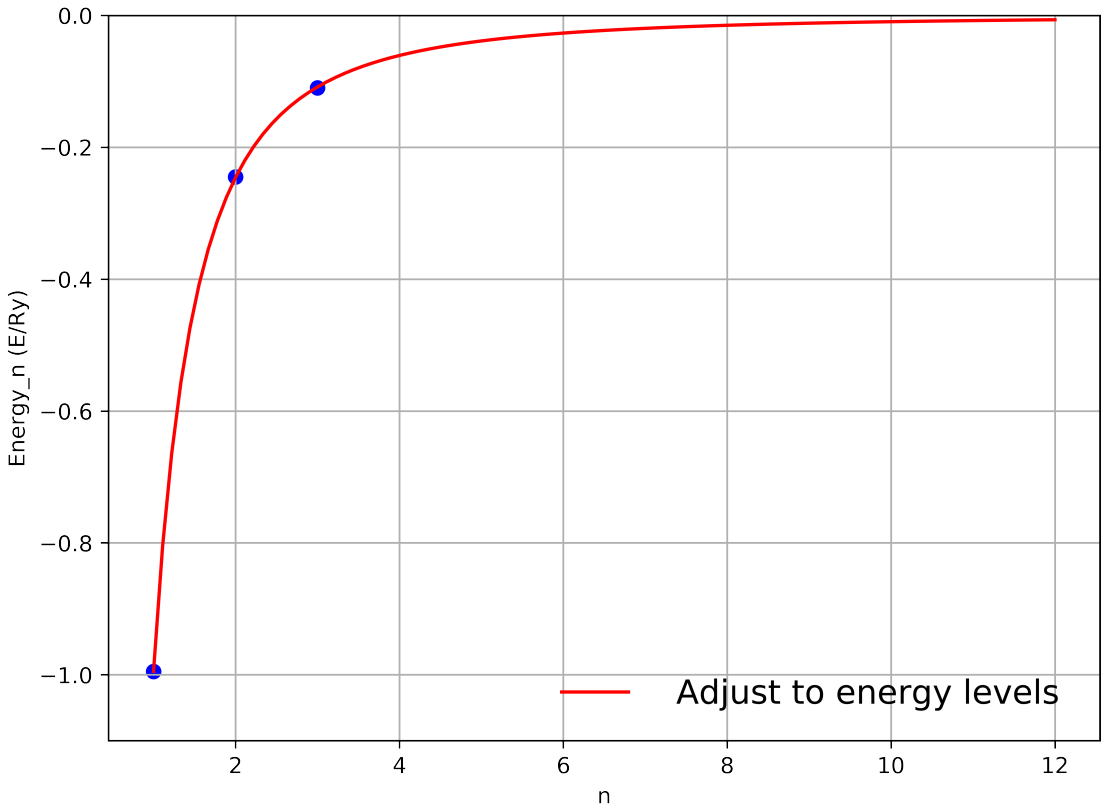

0
−2
−4
−6
−8
−10
Effective Potential
2
4
6
8
10
x




```
 probability normalization
efic1 = 0.033   I1 = 1.950   eI1 = 0.106
efic2 = 0.086   I2 = 5.136   eI2 = 0.168
efic2 = 0.165   I2 = 9.900   eI2 = 0.223

 checking probability
efic1 = 0.033   I1 = 1.000   eI1 = 0.055
efic2 = 0.083   I2 = 0.970   eI2 = 0.032
efic3 = 0.165   I3 = 0.999   eI3 = 0.022

 energy spectrum (E/Ry)   ['-0.995', '-0.245', '-0.110']
 uncertainty in energy (E/Ry)  [' 0.005', ' 0.005', ' 0.005']
 theoretical spectrum (E/Ry)      ['-1.000', '-0.250', '-0.111']
```




```
  energy spectrum (eV)    ['-13.538', '-3.333', '-1.497']
  uncertainty in energy (eV)  [' 0.068', ' 0.068', ' 0.068']
  espectro teorico (eV)      ['-13.606', '-3.401', '-1.512']


   a = -2.016  ea = 0.025    b = -0.005  eb = 0.005       r = 0.999991204      y
= ax + b (y = log|En|, x=log(n))
   alfa = -2.016  e_alfa = 0.025     beta = -0.995  e_beta = 0.005    En (calc)
= -0.995*n**(-2.016)  En (teor) = -1*n**(-2)

<Figure size 432x288 with 0 Axes>
```




```
  theoretical spectrum   (E/Ry): ['-1.000', '-0.250', '-0.111', '-0.062',
'-0.040', '-0.028', '-0.020', '-0.016']
  predicted spectrum  (E/Ry): ['-0.995', '-0.246', '-0.109', '-0.061', '-0.039',
'-0.027', '-0.020', '-0.015']
 predicted uncertainty (eE/Ry): [' 0.005', ' 0.005', ' 0.005', ' 0.005', '
0.005', ' 0.005', ' 0.005', ' 0.005']
```

[ ]:

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