Harmonic_Oscillator

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Part I

One-Dimensional Harmonic Oscillator using Finite Differences

```
%matplotlib inline
```

In [1]:

```
from numpy import identity
```

In [2]:

```
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
```

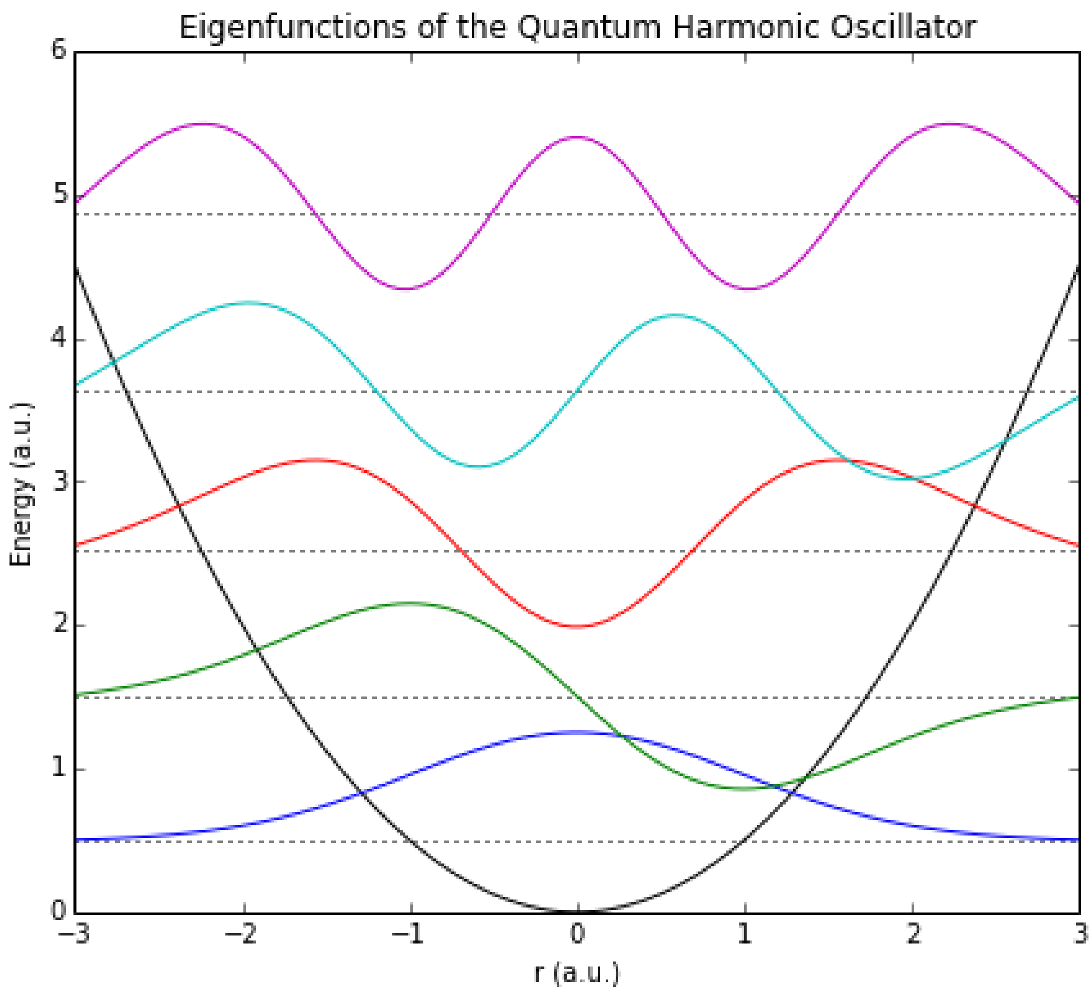
In [3]:

```
from numpy import sqrt

# Normalización de las funciones

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)
#         print j,' integral (sin normalizar) =',rnorm

#       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
```

```
#       Check Normalization
#        suma = 0.0
#        for i in range(1,n):
#             suma = suma + U[i,j]**2
#        print j,' suma=',suma*h

    return
```

In [4]:

```
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 = 100
xmin=-3
xmax=3
x = linspace(xmin,xmax,nsize)
T = array([nsize,nsize])
V = array([nsize,nsize])
H = array([nsize,nsize])
E = array([nsize])

# Oscillator Data
m = 1.0
omega = 1.0

# Kinetic (T) and Potential (V)
T = (-0.5/m)*Laplacian(x)
V = 0.5*(omega**2)*(x**2)

# Hamiltonian
H =  T + diag(V)

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

#define plot size in inches (width, height) & resolution(DPI)
fig = figure(figsize=(7, 6), dpi=100)

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

# Normalization
Normalizate(U,x)

# Plot wavefunctions

for i in range(nfunctions):
    # For each of the first few solutions, plot the energy level:
    axhline(y=E[i],color='k',ls=":")
    # as well as the eigenfunction, displaced by the energy level
    # so they don't all pile up on each other:
    plot(x,U[:,i]+E[i])
axis([xmin,xmax,0,6])
title("Eigenfunctions of the Quantum Harmonic Oscillator")
xlabel("r (a.u.)")
ylabel("Energy (a.u.)")
show()
```



Part II

One-Dimensional Harmonic Oscillator using Special Functions

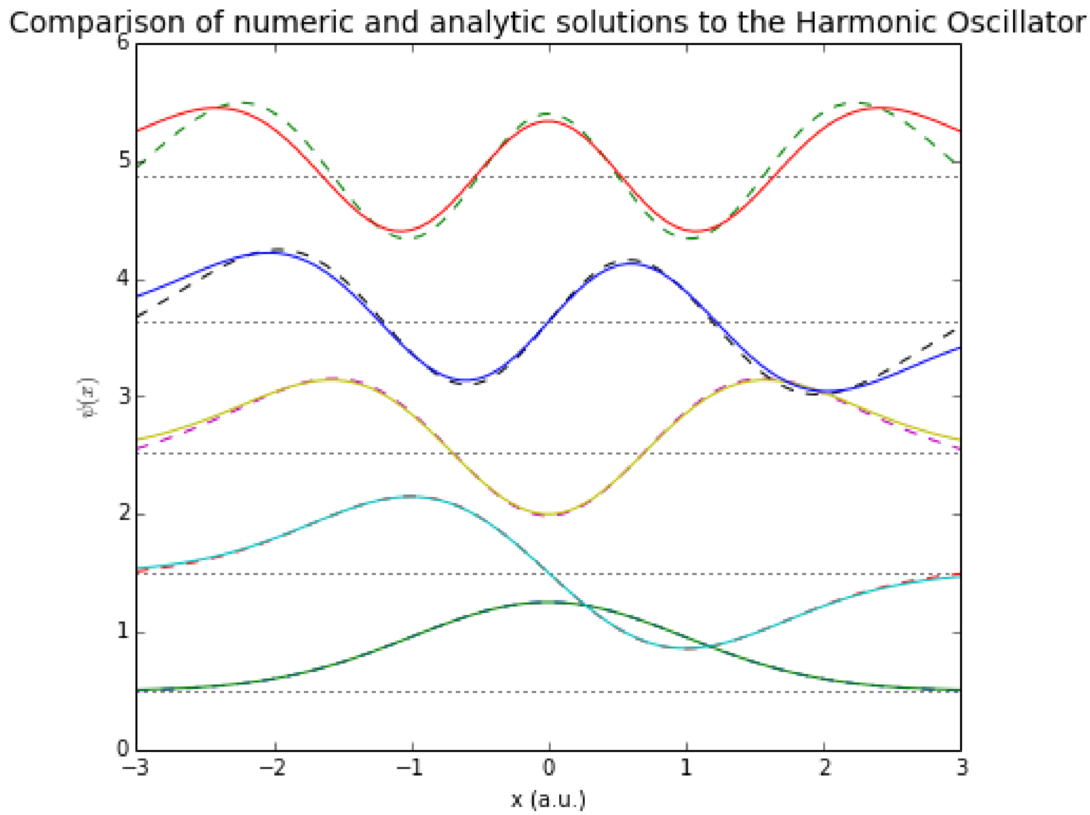
In [5]:

```
from sympy import hermite
from math import gamma, exp, pi, sqrt

# Solución Analítica

def oscillator(n,x):

    arg = 2**n*gamma(n+1)*sqrt(pi)
    psi = 1.0/sqrt(arg) * exp(-x**2/2.0) * hermite(n, x)
    return psi
```

In [6]:

```
from numpy import  linspace , zeros
from matplotlib.pyplot import plot, title, legend, show, axhline, \
                              xlabel, ylabel, axis, figure
```

```
nfunctions = 5

# array definitions
nsize = 100
xmin=-3
xmax=3
x = linspace(xmin,xmax,nsize)
psi = zeros(nsize)

# Plot wavefunctions

#define plot size in inches (width, height) & resolution(DPI)
fig = figure(figsize=(7, 6), dpi=100)

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

    for i in range(0,nsize):
        psi[i] = (-1)**n*oscillator(n,x[i])+E[n]

    plot(x,psi)


xlabel('x (a.u.)')
ylabel(r'$\psi(x)$')
title("Comparison of numeric and analytic solutions to\
 the Harmonic Oscillator",size=14)
#legend()
axis([xmin,xmax,0,6])
show()
```



Chequeo de Normalización (analítico)

In [8]:
```
import numpy as np
import matplotlib as mp
import sympy as sy

from sympy import *

x  = symbols('x ')
k, m, n = symbols('k m n', integer=True)
g1 = symbols('g1', cls=Function)
```

In [9]:
```
def oscillator(n,x):
    psi = 1.0/sqrt((2**n*gamma(n+1)*sqrt(pi))) * exp(-x**2/2.0) * hermite(n, x)
    return psi
```

In [10]:
```
integrate(oscillator(0,x)**2,(x,-oo,oo))
```

Out [10]: 1.00000000000000

In [11]:
```
integrate(oscillator(0,x)*oscillator(3,x),(x,-oo,oo))
```

Out [11]: 0

In [12]:
```
oscillator(1,3.9).evalf()
```

Out [12]: 0.00206292102336555

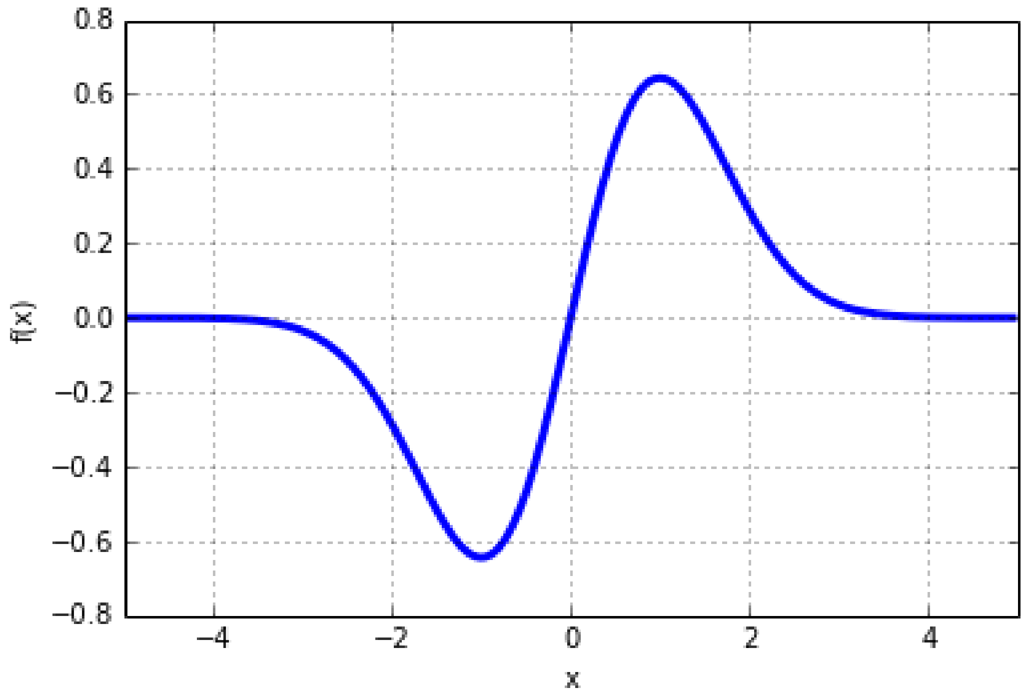
In [13]:
```
g1 = lambda x: oscillator(1,x).evalf()
```

In [14]:
```
for x in range(-5,5):
    print x,g1(x)
```

```
-5 -1.97932226601793e-5
-4 -0.00142538329844946
-3 -0.0354016591068940
-2 -0.287520332179080
-1 -0.644288365113475
0 0
1 0.644288365113475
2 0.287520332179080
3 0.0354016591068940
4 0.00142538329844946
```

In [15]:

```
mpmath.plot(g1,[-5,5])
```



In [ ]:

```
import this
```