## Parte 02 - Deslocamento temporal da função de onda

### a equação da função de onda completa:

$$i\hbar \frac{\partial \Psi}{\partial t} = \text{op } H \Psi$$

### O opH é um operador de evolução temporal. Pode,ele, também assumir, a seguinte identidade matemática:

$$\text{op } U(\Delta t) = e^{\frac{-i \text{ op } H}{\hbar}}$$

### Resultando, portanto, na solução, descrita abaixo:

$$\Psi(x, t + \Delta t) = e^{\frac{-i \text{ op } H\Delta t}{\hbar}} \cdot \Psi(x, t)$$

### Podendo tratar o expoente de um operador, por meio de uma série infinita, tem-se:

$$e^{\frac{-i \text{ op } H\Delta t}{\hbar}} = \sum_n \frac{\left(\frac{-i \text{ op } H\Delta t}{\hbar}\right)^n}{n!}$$

In [12]:
```
#Bibliotecas

import matplotlib.animation as animation
from IPython.display import HTML
import matplotlib.pyplot as plt
import scipy.fftpack as fft
import scipy.linalg as scl
import numpy as np
import math
%matplotlib widget
%matplotlib inline
```

### O Hamiltoniano no espaço:

$x_n = x_0 + n\Delta x$, com $\Delta x = \frac{(x_N - x_0)}{N}$

### Os valores de entrada:

In [16]:
```
hbar = 1
m = 1
```

Processing math: 100%

```
N = 2**11
L = 200.0
step_low = 0.
step_high= 1.
V0 = 10.
```

### Definição do espaço:

In [18]:
```
n = np.arange(N)
x0 = -L/2.
xN = L/2.
Delta_x = (xN - x0)/N
print("Delta_x = ",Delta_x)

x = x0 + n*Delta_x
```

```
Delta_x =  0.09765625
```

### Definição do potencial:

In [20]:
```
V = np.zeros(N)
for i in range(N):
    if x[i]>= step_low and x[i]<= step_high:
        V[i]= V0
```

### Configuração do Hamiltoniano para a função `V`, multiplicação com a matriz inversa:

In [22]:
```
Mdd = 1./(Delta_x**2)*(np.diag(np.ones(N-1),-1)
                      - 2* np.diag(np.ones(N),0)
                      + np.diag(np.ones(N-1),1))
H = -(hbar*hbar)/(2.0*m)*Mdd + np.diag(V)

En,psiT = np.linalg.eigh(H)   # autovalores e os autovetores.
psi = np.transpose(psiT)      # Tomamos a transposta de psiT para os vetores de fun
                              # que podem ser acessados como psi[n]
```

### Intervalo temporal

In [24]:
```
dt_max = 2/np.max(En)      # Critério de estabilidade.
dt = 0.001
if dt > dt_max:
    print("ATENÇÃO: dt está na região instável!")
```

### Função de onda inicial

In [26]:
```
g_x0=-10.
g_k0=6.
g_sig=2.
```

Definição de um Gaussiano no espaço K, com $p = \hbar k$, um momento $k_0$, e o espaço x, $\psi(x,0) = (\frac{2L}{\pi})^{1/4} \cdot e^{-Lx^2}$:

In [28]:
```
def psi0(x,g_x0,g_k0,g_sig):
    _Norm_x=np.sqrt(Delta_x/g_sig)/(np.pi**0.25)

    return(_Norm_x*np.exp(-(x-g_x0)**2/(2.*g_sig*g_sig)+1j*g_k0*x))

psi_t0 = psi0(x,g_x0,g_k0,g_sig)
```

In [29]:
```
# H é Hermitiano?
print("Verifique se H é realmente Hermitiano : ",np.array_equal(H.conj().T,H))
```

```
Verifique se H é realmente Hermitiano :  True
```

In [30]:
```
Ut_mat = np.diag(np.ones(N,dtype="complex128"),0)

print("Criação de uma matriz U(dt = {})".format(dt))
for n in range(1,3):
    # Realiza a soma. Como se trata de matrizes, o processo irá demorar se N for gr
    Ut_mat += np.linalg.matrix_power((-1j*dt*H/hbar),n)/math.factorial(n)
```

```
Criação de uma matriz U(dt = 0.001)
```

In [31]:
```
p = Ut_mat.dot(psi_t0)

print("O quanto a normalização muda por etapa? Desde {} até {}".format(np.linalg.no
print("Nº de etapas em que a norma está errada por um fator 2 : ",1/(np.linalg.norm
```

```
O quanto a normalização muda por etapa? Desde 1.0 até 1.0000000127814086
Nº de etapas em que a norma está errada por um fator 2 :  78238637.96537858
```

### teste do movimento gaussiano:

In [33]:
```
psi_t0 = psi0(x,g_x0,g_k0,g_sig)
psi_t1 = psi_t0
psi_tu = []

for t in range(3500):
    psi_t1 = Ut_mat.dot(psi_t1)
    if t>0 and t%500==0:
        psi_tu.append( (t,psi_t1))
psi_tu.append( (t,psi_t1))
```

### Teste e verificação de coerência dos resultados:

$< E >$ = estado esperado da energia;

$< x >$ = estado esperado da posição

In [35]:
```
print("Normalização : ",np.linalg.norm(psi_tu[-1][1]))

vev_E0=float(np.real(np.sum(np.conjugate(psi_t0)*H.dot(psi_t0))))
```

Processing math: 100%

```python
vev_x0=float(np.real(np.sum(np.conjugate(psi_t0)*x*psi_t0)))

print("<E_(t = 0)> = {:8.4f}  <x_(t = 0)> = {:8.4f}".format(vev_E0,vev_x0))

for t,p in psi_tu:
    norm = np.linalg.norm(p)
    vev_E1 = float(np.real(np.sum(np.conjugate(p)*H.dot(p))))
    vev_x1 = float(np.real(np.sum(np.conjugate(p)*x*p)))
    print("dt = {:7.1f}  norm = {:8.5f}  <E> = {:8.4f}  <x_(dt)> = {:8.4g}".format(
```

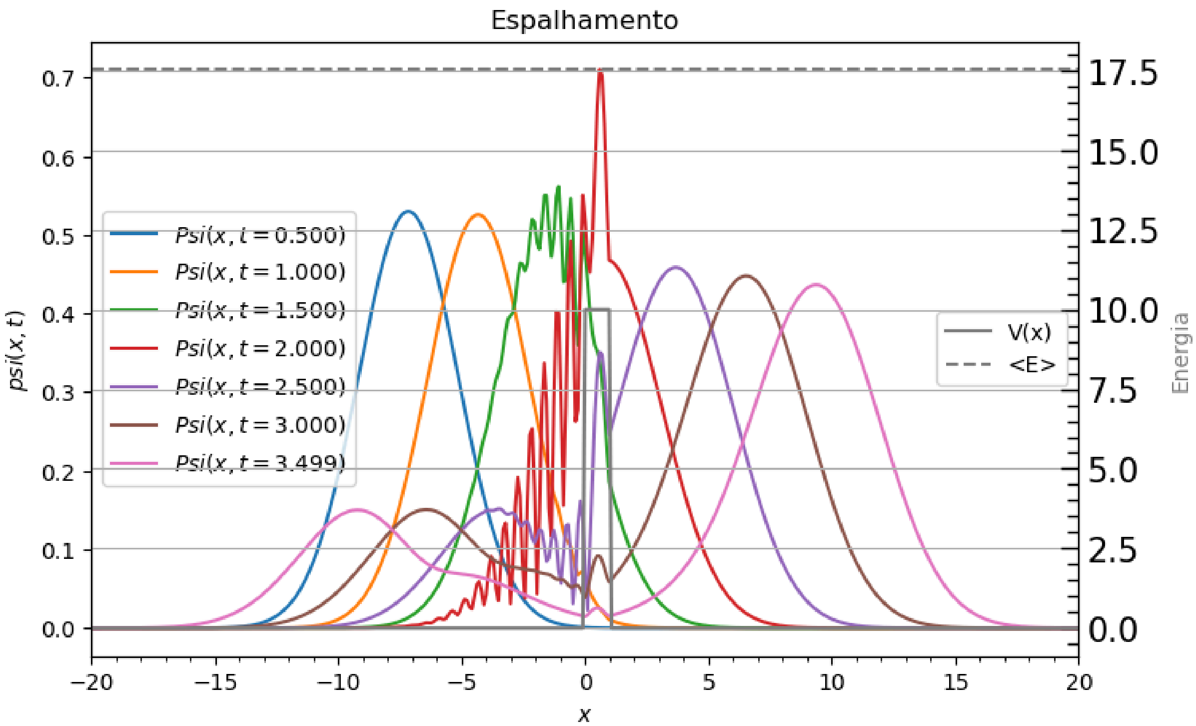
```
Normalização :  1.000044736361259
<E_(t = 0)> =  17.5429  <x_(t = 0)> = -10.0000
dt =   500.0  norm =  1.00001  <E> =  17.5432  <x_(dt)> =   -7.164
dt =  1000.0  norm =  1.00001  <E> =  17.5434  <x_(dt)> =   -4.335
dt =  1500.0  norm =  1.00002  <E> =  17.5436  <x_(dt)> =    -1.55
dt =  2000.0  norm =  1.00003  <E> =  17.5439  <x_(dt)> =   0.8044
dt =  2500.0  norm =  1.00003  <E> =  17.5441  <x_(dt)> =     2.91
dt =  3000.0  norm =  1.00004  <E> =  17.5443  <x_(dt)> =    5.103
dt =  3499.0  norm =  1.00004  <E> =  17.5446  <x_(dt)> =    7.305
```

### Dos dados obtidos, resulta:

In [37]:

```python
def opt_plot():
    plt.minorticks_on()
    plt.tick_params(axis='both',which='minor', direction = "in",
                    top = True,right = True, length=5,width=1,
                    labelsize=15)
    plt.tick_params(axis='both',which='major', direction = "in",
                    top = True,right = True, length=8,width=1,
                    labelsize=15)



plt.figure(figsize=(8,5))

if vev_E0>max(V):
    plt.title('Espalhamento')
else:
    plt.title('Tunelamento')
plt.ylabel('$psi(x,t)$')
plt.xlabel('$x$')
# plt.plot(x,np.abs(psi_t0)/np.sqrt(Delta_x),label="$\Psi(x,t=0)$")

for t,p in psi_tu:

    plt.plot(x,np.abs(p)/np.sqrt(Delta_x),label="$Psi(x,t={:6.3f})$".format(t*dt))
    plt.legend(loc = 'center left')

ax1 = plt.twinx()
plt.plot(x,V,color="grey",label="V(x)")
plt.plot([x[0],x[N-1]],[vev_E0,vev_E0],color="grey",linestyle="--",label="<E>")
plt.ylabel("Energia",color="grey")
plt.xlim(g_x0-5*g_sig,-g_x0+5*g_sig)
plt.legend(loc='best')
plt.grid()
opt_plot()
```

```
plt.savefig('Estado deslocado.png')
```




In [38]:
```
%time Ut_05s = np.linalg.matrix_power(Ut_mat,int(0.5/dt) )
```

```
CPU times: total: 2min
Wall time: 1min 15s
```

## Repetição de tarefa

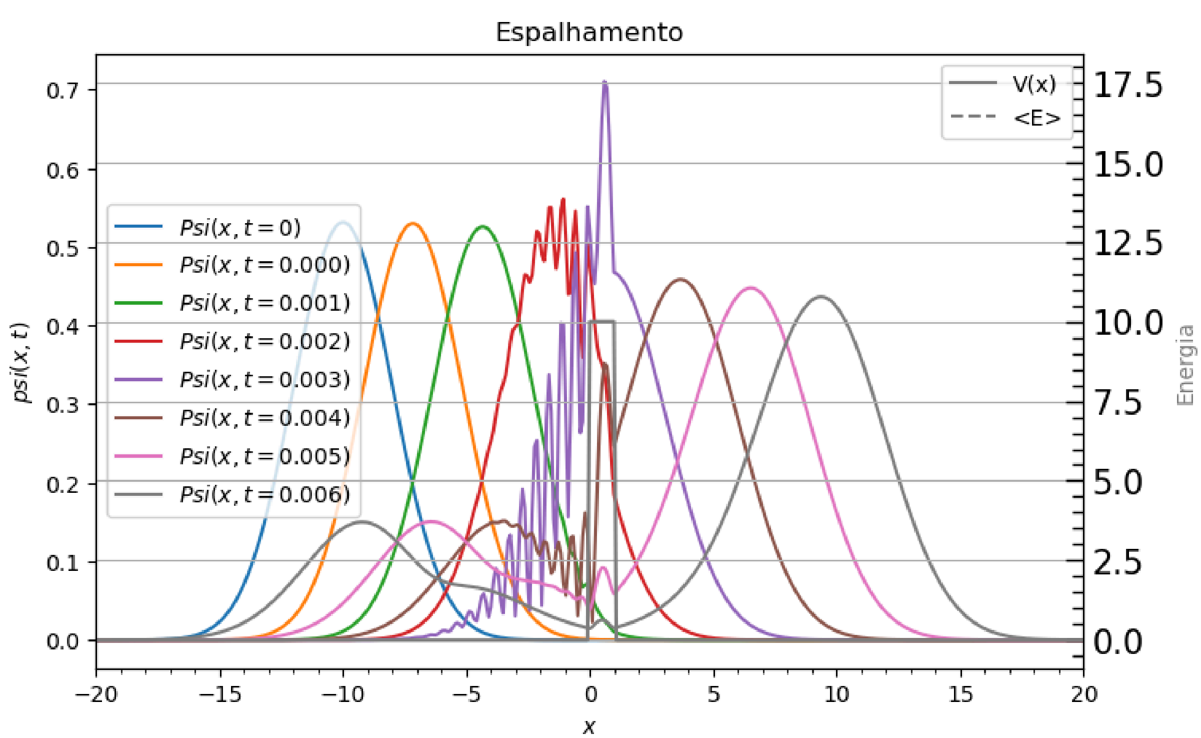
In [40]:
```
psi_t0 = psi0(x,g_x0,g_k0,g_sig)
psi_t1 = psi_t0
psi_tu05 = []

for t in range(7):
    psi_t1 = Ut_05s.dot(psi_t1)
    psi_tu05.append( (t,psi_t1))
    # psi_tu.append( (t,psi_t1))
print("Start")
v1=[]
v2=[]
tm=[]
count=0
for t,p in psi_tu05:
    norm = np.linalg.norm(p)
    vev_E1 = float(np.real(np.sum(np.conjugate(p)*H.dot(p))))
    vev_x1 = float(np.real(np.sum(np.conjugate(p)*x*p)))
    v1.append(vev_E1)

    v2.append(vev_x1)
    tm.append(count)
    count=count+1
    print("dt = {:7.1f}  norm = {:8.5f}  <E> = {:8.4f}  <x_(dt)> = {:8.4g}".format(
```

Processing math: 100%

```
Start
dt =     0.0  norm =  1.00001  <E> =  17.5432  <x_(dt)> =    -7.17
dt =     1.0  norm =  1.00001  <E> =  17.5434  <x_(dt)> =    -4.34
dt =     2.0  norm =  1.00002  <E> =  17.5436  <x_(dt)> =   -1.555
dt =     3.0  norm =  1.00003  <E> =  17.5439  <x_(dt)> =   0.8002
dt =     4.0  norm =  1.00003  <E> =  17.5441  <x_(dt)> =    2.905
dt =     5.0  norm =  1.00004  <E> =  17.5443  <x_(dt)> =    5.099
dt =     6.0  norm =  1.00004  <E> =  17.5446  <x_(dt)> =    7.305
```

In [41]:

```
plt.figure(figsize=(8,5))

if vev_E0>max(V):
    plt.title('Espalhamento')
else:
    plt.title('Tunelamento')
plt.ylabel('$psi(x,t)$')
plt.xlabel('$x$')
line, = plt.plot(x,np.abs(psi_t0)/np.sqrt(Delta_x),label="$Psi(x,t=0)$")

for t,p in psi_tu05:
    plt.plot(x,np.abs(p)/np.sqrt(Delta_x),label="$Psi(x,t={:6.3f})$".format(t*dt))
    plt.legend(loc='center left')

ax1 = plt.twinx()
plt.plot(x,V,color="grey",label="V(x)")
plt.plot([x[0],x[6]],[vev_E0,vev_E0],color="grey",linestyle="--",label="<E>")
plt.ylabel("Energia",color="grey")
plt.xlim(g_x0-5*g_sig,-g_x0+5*g_sig)
plt.legend(loc='best')
plt.grid()
opt_plot()

plt.savefig('Estado deslocado - Pré-computados.png')
```




Processing math: 100%

# Parte 3 - A Regressão Simbólica

In [43]:
```
from sklearn.utils import check_random_state, shuffle
from gplearn.genetic import SymbolicRegressor
from sklearn.ensemble import RandomForestRegressor
from sklearn.tree import DecisionTreeRegressor
from sklearn.utils.random import check_random_state
from mpl_toolkits.mplot3d import Axes3D
from IPython.display import Image
import pydot
import graphviz
from sympy import *
import pandas as pd
```

## Definição dos Operadores

In [45]:
```
converter = {
    'sub': lambda x, y : x - y,
     'div': lambda x, y : x/y,
    'mul': lambda x, y : x*y,
    'add': lambda x, y : x + y,
    'neg': lambda x    : -x,
    'pow': lambda x, y : x**y,
    'sin': lambda x    : sin(x),
    'cos': lambda x    : cos(x),
    'inv': lambda x: 1/x,
    'sqrt': lambda x: x**0.5,
    'pow3': lambda x: x**3
}
```

### Interpretação Probabilística Gaussiana da Distribuição Normal

$$N(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot e^{-\frac{1}{2}\frac{(x-\mu)}{\sigma}^2}$$

:

In [47]:
```
m1=[]
md=[]
count=0
tem=0
df=pd.DataFrame()
df2=pd.DataFrame()
xix=[]
df['v1']=v1
df2['v2']=v2

for i in v2:
    m1.append(i)
    tem=i-vev_x0
    md.append(tem**2)
```

Processing math: 100%

```
df['m1']=md
df2['t']=tm



dp=2.83/3
A = [float(i) for i in m1]
for i in A:
    xix=np.linspace(-(3.*dp),(3.*dp),40)
    y=0.39*(2.76**(-0.5*(xix**2)))
```

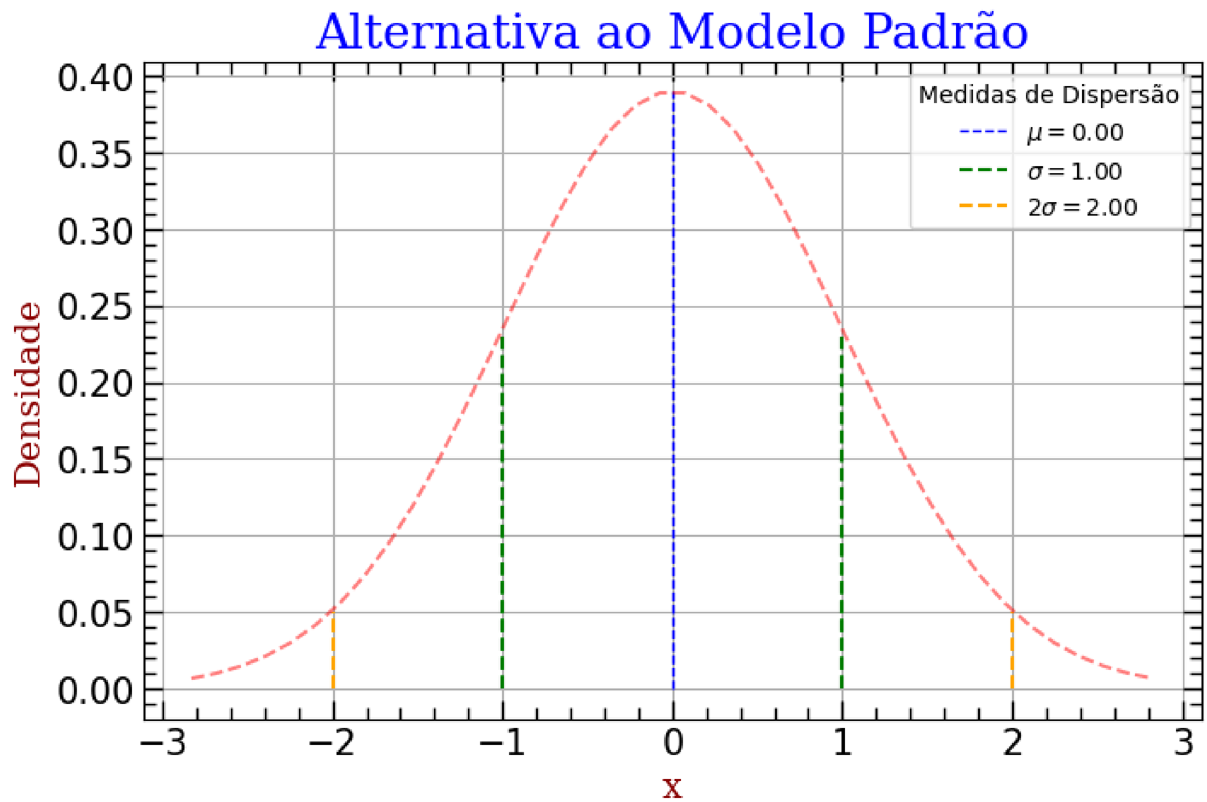
## A amostra acima, resulta:

In [49]:
```
def opt_plot():
    plt.minorticks_on()
    plt.tick_params(axis='both',which='minor', direction = "in",
                    top = True,right = True, length=5,width=1,
                    labelsize=15)
    plt.tick_params(axis='both',which='major', direction = "in",
                    top = True,right = True, length=8,width=1,
                    labelsize=15)
plt.figure(figsize=(8,5))

textstr = '\n'.join((
    r'$\mu=%.2f$' % (0, ),
    ))

textstr02 = '\n'.join((
    r'$\sigma=%.2f$' % (1, ),
))

textstr03 = '\n'.join((
    r'$\sigma=%.2f$' % (2, ),
))

textstr04 = '\n'.join((
    r'$\sigma=%.2f$' % (1, ),
    r'$\mu=%.2f$' % (0, ),
))

plt.vlines(0, 0, 0.39, linestyle='dashed', color='b', linewidth=1, label=str(textst
plt.vlines(1, 0, 0.23, linestyle='dashed', color='green', linewidth=1.5, label= str
plt.vlines(-1, 0, 0.23, linestyle='dashed', color='green', linewidth=1.5) # vlines(
plt.vlines(2, 0, 0.05, linestyle='dashed', color='orange', linewidth=1.5, label= '2
plt.vlines(-2, 0, 0.05, linestyle='dashed', color='orange', linewidth=1.5) # vlines

font1 = {'family':'serif','color':'blue','size':20}
font2 = {'family':'serif','color':'darkred','size':15}

plt.title("Alternativa ao Modelo Padrão", fontdict = font1)
plt.xlabel("x", fontdict = font2)
plt.ylabel("Densidade", fontdict = font2)

plt.legend(title='Medidas de Dispersão')
plt.grid()
```

Processing math: 100%

```
opt_plot()
plt.plot(xix,y ,'r--', alpha=0.5, label= textstr04)
```

Out[49]: [<matplotlib.lines.Line2D at 0x21c95f5cda0>]




## Criação e Calibração de um modelo Simbólico Regressor:

In [51]:
```
function_set = ['add', 'sub', 'mul', 'div','cos','sin','neg','inv']
# Instanciação
est_gp = SymbolicRegressor(population_size=5000,
                           generations=20,function_set=function_set,
                           stopping_criteria=0.01,
                           p_crossover=0.7, p_subtree_mutation=0.1,
                           p_hoist_mutation=0.05, p_point_mutation=0.1,
                           max_samples=0.9, verbose=1,
                           parsimony_coefficient=0.01, random_state=0)
# Ajuste
est_gp.fit(xix.reshape(-1, 1),y)
```

```
    |   Population Average    |             Best Individual              |
---- ------------------------- ------------------------------------------ ----------
 Gen   Length          Fitness   Length          Fitness      OOB Fitness  Time Left
   0    15.94          8.42754       24         0.101256         0.141842      2.44m
   1     8.38          1.41838       10        0.0282817        0.0287366      2.23m
   2     4.25         0.913171       10        0.0275074        0.0357058      1.91m
   3     2.38         0.458598       10        0.0262319        0.0471853      1.68m
   4     2.34          69.5123       10        0.0262295        0.0472067      1.63m
   5     4.42          1.11605       11        0.0181481        0.0271488      1.57m
   6     6.21          1.40624       11        0.0183373        0.0356987      1.49m
   7     6.89          1.00531       11        0.0196629        0.0237683      1.53m
   8     7.20          0.86294       11        0.0185499        0.0337846      1.25m
   9     7.36         0.927227       12        0.0193277        0.0303689      1.22m
  10     7.54          1.14538       12        0.0202671        0.0219142      1.07m
  11     7.90          1.22699        8        0.0258667         0.038024     56.28s
  12     8.04          1.22625        8        0.0252462        0.0436084      1.06m
  13     7.96          1.29076        8        0.0249788        0.0460152      1.05m
  14     7.86          1.30819        8        0.0245602          0.04586     55.62s
  15     8.06          1.22489        8        0.0247419        0.0481478     38.25s
  16     7.99          1.55607        8        0.0246505          0.04897     22.28s
  17     7.92          1.26517       11        0.0241093        0.0259531     17.71s
  18     7.97          1.25025        8        0.0246505          0.04897     11.49s
  19     8.00           1.2177       10         0.023813        0.0384339      0.00s
```

Out[51]:

```
SymbolicRegressor
div(0.333, sub(0.812, neg(mul(mul(0.696, X0), X0))))
```

### Escore:

In [53]:

```python
print('R2:',est_gp.score(xix.reshape(-1, 1),y))
next_e = sympify(str(est_gp._program), locals=converter)
y1=next_e
```

```
R2: 0.9502743138806782
```

### Equação Proposta:

In [55]:

```python
y1
```

Out[55]:

$$\frac{0.333}{0.696X_0^2 + 0.812}$$

## Soluções para o Poço de Potencial Infinito

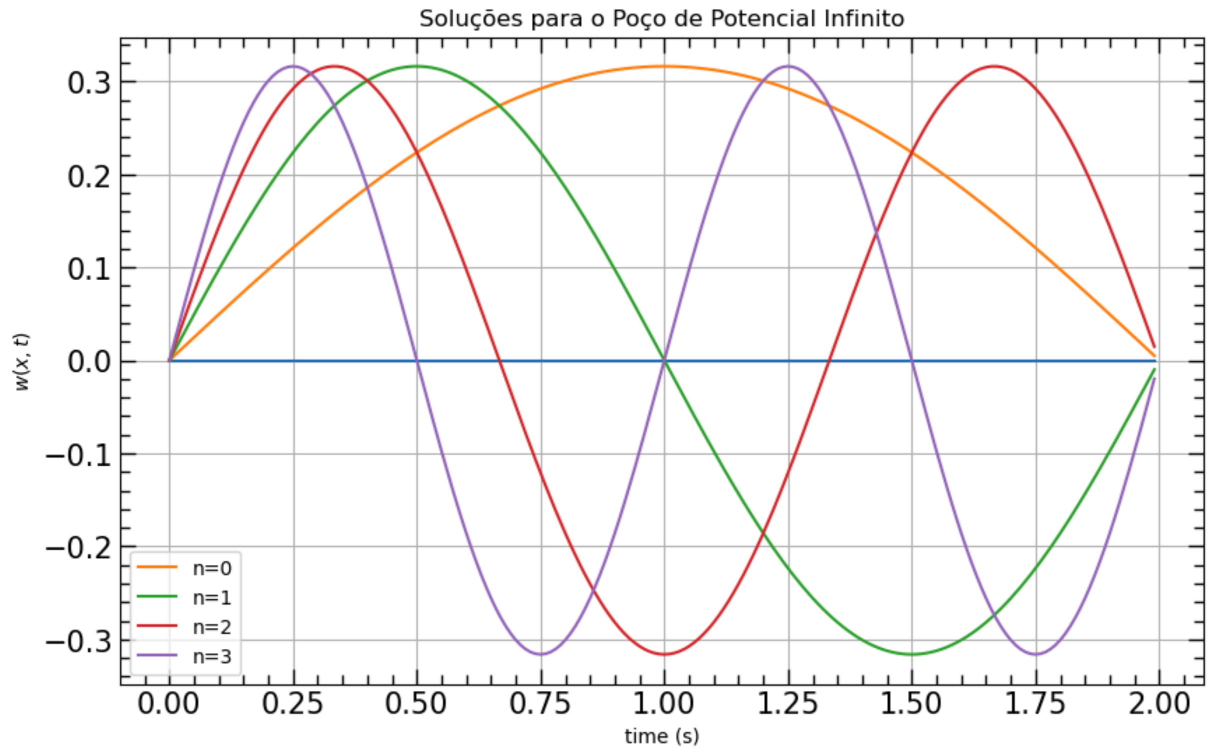
### Solução da função de onda da posição

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

Processing math: 100%

In [58]:

```
import matplotlib.pyplot as plt
import numpy as np
def opt_plot():
    plt.minorticks_on()
    plt.tick_params(axis='both',which='minor', direction = "in",
                    top = True,right = True, length=5,width=1,
                    labelsize=15)
    plt.tick_params(axis='both',which='major', direction = "in",
                    top = True,right = True, length=8,width=1,
                    labelsize=15)



a=20
A=np.sqrt(2/a)
# Data for plotting
for i in range(5):
    t = np.arange(0.0, 2.0, 0.01)
    s = A*np.sin(0 * np.pi * t)
s1 = A*+np.sin(0.5 * np.pi * t)
s2 = A*np.sin(1.0 * np.pi * t)
s3 = A*np.sin(1.5 * np.pi * t )
s4 = A*np.sin(2.0 * np.pi * t)


fig, ax = plt.subplots(figsize=(10,6))


ax.plot(t, s)
ax.plot(t, s1,label='n=0')
ax.plot(t, s2,label='n=1')
ax.plot(t, s3,label='n=2')
ax.plot(t, s4,label='n=3')


ax.set(xlabel='time (s)', ylabel='$w(x,t)$',
       title="Soluções para o Poço de Potencial Infinito")
ax.grid()
opt_plot()

plt.legend()

fig.savefig("test.png")
plt.show()
```




### Gera-se e ajusta-se,um modelo Simbólico Regressor para a solução da função de onda da Posição:

In [60]:
```
est_gp.fit(t.reshape(-1, 1),s1)
```

```
    |   Population Average    |             Best Individual              |
---- ------------------------- ------------------------------------------ ----------
 Gen   Length          Fitness   Length          Fitness      OOB Fitness  Time Left
   0    15.94          10.9162        6        0.0305686        0.0286007      2.70m
   1     8.25          1.36407        9        0.0238001        0.0246281      2.65m
   2     5.03         0.916274        9        0.0248264        0.0153917      2.21m
   3     2.76         0.458664        7        0.0265144         0.031241      2.49m
   4     2.38          16.2677        7         0.026512        0.0312625      1.71m
   5     5.04         0.628504        6        0.0142702           0.0251      1.70m
   6     6.00          1.07399        6        0.0145615        0.0224778      1.70m
   7     6.08         0.645816        6        0.0137287        0.0299735      1.32m
   8     6.07         0.686379        6         0.013608        0.0310599      1.25m
   9     6.19         0.767054        6        0.0124938        0.0410876      1.33m
  10     6.10         0.799589        6        0.0129802        0.0367098      1.44m
  11     6.08         0.641764        6         0.013121        0.0354423      1.09m
  12     6.19         0.677095        6        0.0122761        0.0430471     58.81s
  13     6.17         0.895997        6         0.012991        0.0366123     38.97s
  14     6.06         0.736398        6        0.0132391          0.03438     32.38s
  15     6.18         0.696137        6        0.0133269        0.0335893     26.38s
  16     6.17         0.844118        6        0.0132413        0.0343599     20.57s
  17     6.09         0.700994        6        0.0128263        0.0380947     13.77s
  18     6.16         0.612862        6        0.0130871        0.0357479      6.65s
  19     6.17         0.633526        6        0.0125276        0.0407834      0.00s
```

Out[60]:

SymbolicRegressor

add(mul(-0.517, X0), sin(X0))

### Escore

In [62]:
```
print('R2:',est_gp.score(t.reshape(-1, 1),s1))
next_e = sympify(str(est_gp._program), locals=converter)
y2=next_e
```

```
R2: 0.9048979343134357
```

## Equação Proposta

In [64]:
```
y2
```

Out[64]:

$-0.517X_0 + \sin\left(X_0\right)$

### Solução para o espectro energético

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

### Verificando os níveis de energia:

In [66]:
```
import numpy as np
a=1
h=1
m=1
En=0
Enn=[]
for i in range(7):
    En=((i**2)*(h**2)*(np.pi**2))/(2*m*a*a)
    Enn.append(En)

for i in range(7):
    n = i+1
    print("E[{}] = {:9.4f}".format(n,Enn[i],n, n*n*np.pi**2*h*h/(2*m*a*a)))
```

```
E[1] =    0.0000
E[2] =    4.9348
E[3] =   19.7392
E[4] =   44.4132
E[5] =   78.9568
E[6] =  123.3701
E[7] =  177.6529
```

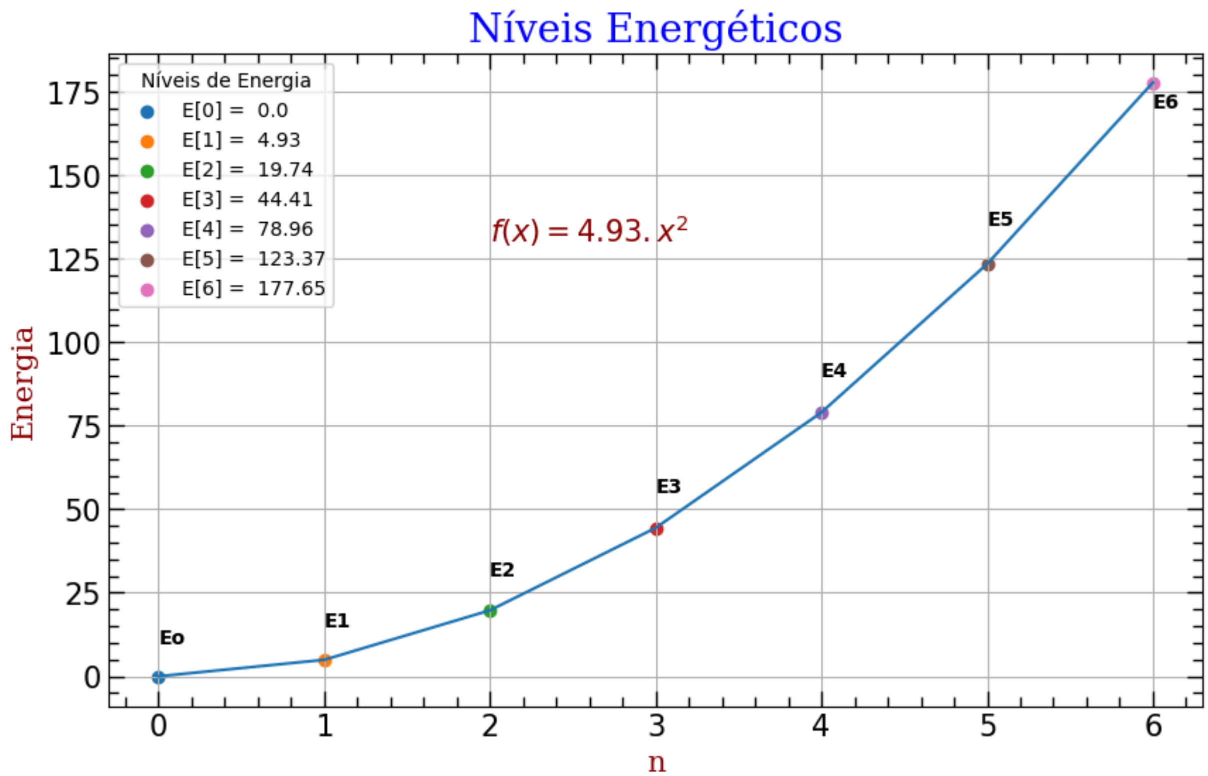
### Gráfico da Energia Quantizada:

In [68]:
```
def opt_plot():
    plt.minorticks_on()
```

Processing math: 100%

```
    plt.tick_params(axis='both',which='minor', direction = "in",
                    top = True,right = True, length=5,width=1,
                    labelsize=15)
    plt.tick_params(axis='both',which='major', direction = "in",
                    top = True,right = True, length=8,width=1,
                    labelsize=15)

plt.figure(figsize=(10, 6))
plt.plot(Enn)
plt.text(x=0.0, y=10, s="Eo", weight="bold")
plt.text(x=1.0, y=15, s="E1", weight="bold")
plt.text(x=2.0, y=30, s="E2", weight="bold")
plt.text(x=3.0, y=55, s="E3", weight="bold")
plt.text(x=4.0, y=90, s="E4", weight="bold")
plt.text(x=5.0, y=135, s="E5", weight="bold")
plt.text(x=6.0, y=170, s="E6", weight="bold")

for i in range(7):
    En=((i**2)*(h**2)*(np.pi**2))/(2*m*a*a)

    plt.scatter(i,En, marker='o',label="E["+str(i)+"] =  "+str(round(Enn[i],2)))

font1 = {'family':'serif','color':'blue','size':20}
font2 = {'family':'serif','color':'darkred','size':15}

plt.title("Níveis Energéticos", fontdict = font1)
plt.xlabel("n", fontdict = font2)
plt.ylabel("Energia", fontdict = font2)
plt.text(x=2.0, y=130, s=r'$f(x) = 4.93.{x^2}$',fontdict = font2)

plt.legend(title='Níveis de Energia')
opt_plot()

plt.grid()
```

Processing math: 100%




**Para:**

In [70]:
```
l_count=np.linspace(0,6,7)
E_df=np.array([l_count,Enn])
E_df02=E_df.T
E_df02
y_E=4.93*E_df[:,0]**2
```

## Obtem-se o seguinte modelo:

In [72]:
```
function_set = ['add', 'sub', 'mul', 'div','cos','sin','neg','inv']
# Instanciação
est_gp = SymbolicRegressor(population_size=5000,
                           generations=20,function_set=function_set,
                           stopping_criteria=0.01,
                           p_crossover=0.7, p_subtree_mutation=0.1,
                           p_hoist_mutation=0.05, p_point_mutation=0.1,
                           max_samples=0.9, verbose=1,
                           parsimony_coefficient=0.01, random_state=0)
# Ajuste
est_gp.fit(E_df,y_E)
```

```
    |   Population Average    |             Best Individual              |
---- ------------------------- ------------------------------------------ ----------
 Gen   Length          Fitness   Length          Fitness      OOB Fitness  Time Left
   0    10.86      1.23511e+07       14                0                0      2.06m
```

Processing math: 100%

Out[72]:

SymbolicRegressor

```
neg(neg(div(mul(inv(X0), mul(X1, -0.362)), sub(cos(X2), sin(0.200)))))
```

### Cujo Escore é:

In [74]:
```
next_e = sympify(str(est_gp._program), locals=converter)
y3=next_e
```

### com a proposta de equação:

In [76]:
```
y3
```

Out[76]:

$$-\frac{0.362X_1}{X_0\left(\cos\left(X_2\right)-0.198669330795061\right)}$$

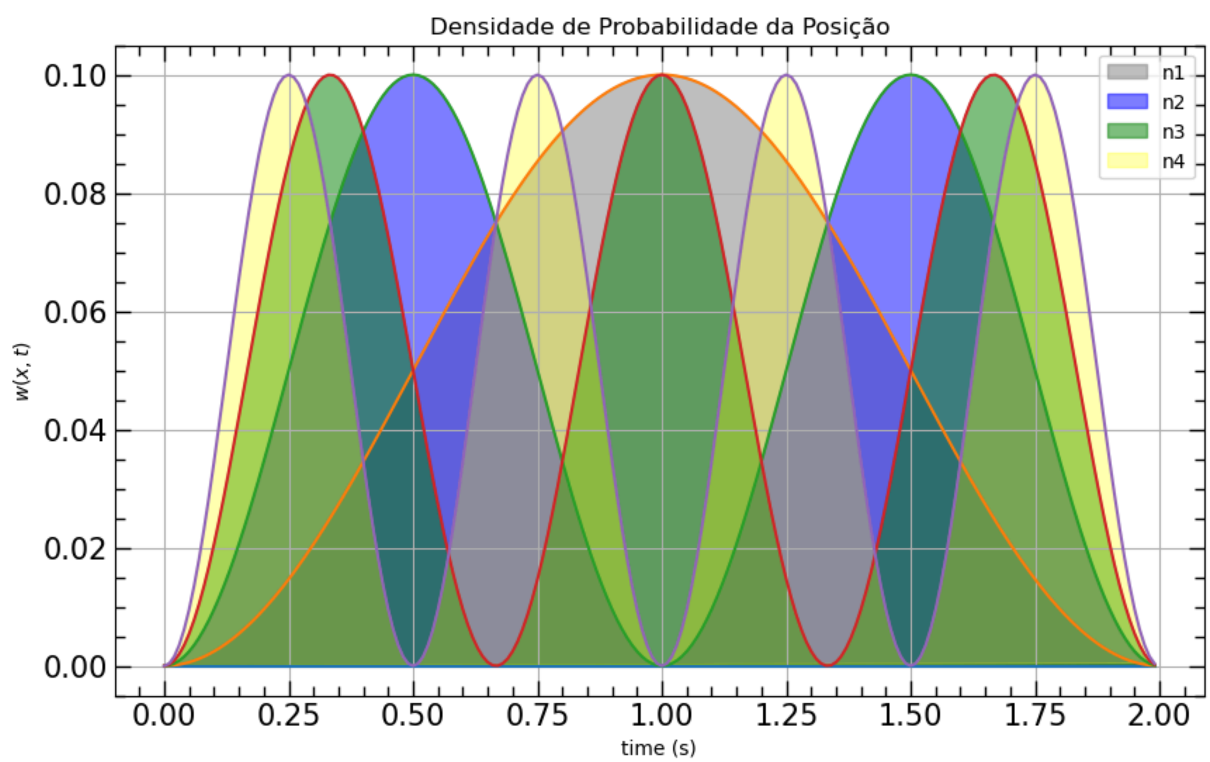
## Densidade de Probabilidade da posição

$$|\psi_n(x)|^2=\frac{2}{a}\sin^2(n\pi x)$$

In [78]:
```
import matplotlib.pyplot as plt
import numpy as np

def opt_plot():
    plt.minorticks_on()
    plt.tick_params(axis='both',which='minor', direction = "in",
                    top = True,right = True, length=5,width=1,
                    labelsize=15)
    plt.tick_params(axis='both',which='major', direction = "in",
                    top = True,right = True, length=8,width=1,
                    labelsize=15)

val_esp=[-7.17,-4.344,-1.555,0.8002,2.905,5.095 ,7.305]

a=20
A=(2/a)
# Data for plotting
t = np.arange(0.0, 2.0, 0.01)
x=np.arange(0.0,2.0,0.01)


s = A*(np.sin((0 * np.pi * x)))**2

s1 = A*(np.sin((0.5 * np.pi * abs(x))))**2
s2 = A*(np.sin((1.0 * np.pi * x)))**2
s3 = A*(np.sin((1.5 * np.pi * x)))**2
s4 = A*(np.sin((2.0 * np.pi * x)))**2
```

Processing math: 100%

```
fig, ax = plt.subplots(figsize=(10,6))
ax.plot(x, s)

ax.plot(x, s1)
ax.fill(x,s1,color='grey', alpha=0.5, label='n1')
ax.plot(x, s2)
ax.fill(x,s2,color='blue', alpha=0.5, label='n2')
ax.plot(x, s3)
ax.fill(x,s3,color='green', alpha=0.5, label='n3')
ax.plot(x, s4)
ax.fill(x,s4,color='yellow', alpha=0.3, label='n4')



ax.set(xlabel='time (s)', ylabel='$w(x,t)$',
       title="Densidade de Probabilidade da Posição")
ax.grid()
ax.legend()
opt_plot()

fig.savefig("test.png")
plt.show()
```




## Relaciona-se os valores médios esperados, da funçao de onda, com a função normal gaussiana:

In [80]:

```
val_esp=np.array([-7.17,-4.344,-1.555,0.8002,2.905,5.095 ,7.305])
niveis=[0,1,2,3,4,5,6]
arr_value=np.array([[niveis],[val_esp]])
x_arr = val_esp
print(x_arr)
y_arr=0.399*(2.76**(-0.5*x_arr[:]**2))
```

```
[-7.17   -4.344  -1.555   0.8002  2.905   5.095   7.305 ]
```

### para então, modular:

In [82]:
```
function_set = ['add', 'sub', 'mul', 'div','cos','sin','neg','inv']
# Instanciação
est_gp = SymbolicRegressor(population_size=5000,
                           generations=20,function_set=function_set,
                           stopping_criteria=0.01,
                           p_crossover=0.7, p_subtree_mutation=0.1,
                           p_hoist_mutation=0.05, p_point_mutation=0.1,
                           max_samples=0.9, verbose=1,
                           parsimony_coefficient=0.01, random_state=0)
# Ajuste
est_gp.fit(x_arr.reshape(-1,1),y_arr)
```

```
    |   Population Average    |             Best Individual              |
---- ------------------------- ------------------------------------------ ----------
 Gen   Length          Fitness   Length          Fitness      OOB Fitness  Time Left
   0    15.94          24.2581        9        0.0150923         0.125521      2.32m
   1     9.25          3.10342       29         0.001741         0.390678      2.51m
```

Out[82]:

SymbolicRegressor

```
sin(mul(cos(sub(sin(add(0.782, 0.138)), sin(sub(0.773, X0)))), div(cos(inv
(cos(X0))), sub(sin(add(-0.483, 0.614)), mul(mul(X0, X0), add(X0, X0))))))
```

### Escore:

In [84]:
```
print('R2:',est_gp.score(x_arr.reshape(-1,1),y_arr))
next_e = sympify(str(est_gp._program), locals=converter)
y2_arr=next_e
```

```
R2: -1.099778938698206
```

### Equaçao:

In [86]:
```
y2_arr
```

Out[86]:

$$\sin\left(\frac{\cos\left(\sin\left(X_0 - 0.773\right) + 0.795601620036366\right)\cos\left(\frac{1}{\cos\left(X_0\right)}\right)}{0.130625639531083 - 2X_0^3}\right)$$

### O desvio padrão da posição:

$$\Delta xn = \sqrt{< x^2 n > \; - \; < xn >^2} = a\sqrt{\frac{1}{12} - \frac{1}{2\pi^2 n^2}}$$

Processing math: 100%

In [88]:

```
import pandas as pd
xx0=-10
val_esp=[-7.17,-4.344,-1.555,0.8002,2.905,5.095 ,7.305]
a=val_esp[6]-val_esp[0]
x_quadrado=0
dp=[]
n=1
desp=0
j=-10

c=0
dsp=[]
for i in val_esp:
    if (j<0 and i>0):
        c=np.abs(j)+i
    else:
        c=np.abs(j)-np.abs(i)
        c=np.abs(c)
    dsp.append(c)
    j=i
dsp
er_count=0
err=[]
med_ex=2.86
for i in dsp:
    er_count=med_ex-i
    err.append(er_count)
err
dpp=pd.DataFrame()
dpp['DesvioP']=dsp
dpp['ErrDesvioP']=err

dpp
```

Out[88]:

| | DesvioP | ErrDesvioP |
|---|---|---|
| **0** | 2.8300 | 0.0300 |
| **1** | 2.8260 | 0.0340 |
| **2** | 2.7890 | 0.0710 |
| **3** | 2.3552 | 0.5048 |
| **4** | 2.1048 | 0.7552 |
| **5** | 2.1900 | 0.6700 |
| **6** | 2.2100 | 0.6500 |

Podemos encontrar, também, o desvio padrão do momento

$$e^{\frac{-i\ \text{op}\ H\Delta t}{\hbar}} = \sum_n \frac{\left(\frac{-i\ \text{op}\ H\Delta t}{\hbar}\right)^n}{n!}$$

$$\Delta Kn =< K^2 n > - < Kn >^2 = \frac{n\hbar}{a}$$

In [90]:
```
import numpy as np
a=20

h=1
dpm=0
dmp=[]
for i in range(7):
    a=np.abs(a)
    dpm=(i*np.pi)/a
    dmp.append(dpm)
```

## O Princípio da Incerteza

$$\Delta x.\,\Delta p > \frac{\hbar}{2}$$

In [92]:
```
desvf=pd.DataFrame()
desvf["dp"]=dpp.DesvioP
desvf["dmp"]=dmp
j=0
incerteza=[]
form=[]
f=r'$\Delta x.\Delta p $'
g=r'$\Delta x $'
h=r'$\Delta p $'
c=0
gord=dpp.DesvioP
hord=dmp
for i in dpp.DesvioP:
   j=dmp[c]*i
   incerteza.append(j)
   form.append(f)


   c=c+1
desvf02=pd.DataFrame()
desvf02[g]=gord
desvf02[h]=hord
desvf02["lesquerdo"]=form
desvf02["incerteza"]=incerteza
desvf02
```

Processing math: 100%

Out[92]:

| | $\Delta x$ | $\Delta p$ | Iesquerdo | incerteza |
|---|---|---|---|---|
| **0** | 2.8300 | 0.000000 | $\Delta x.\Delta p$ | 0.000000 |
| **1** | 2.8260 | 0.157080 | $\Delta x.\Delta p$ | 0.443907 |
| **2** | 2.7890 | 0.314159 | $\Delta x.\Delta p$ | 0.876190 |
| **3** | 2.3552 | 0.471239 | $\Delta x.\Delta p$ | 1.109862 |
| **4** | 2.1048 | 0.628319 | $\Delta x.\Delta p$ | 1.322485 |
| **5** | 2.1900 | 0.785398 | $\Delta x.\Delta p$ | 1.720022 |
| **6** | 2.2100 | 0.942478 | $\Delta x.\Delta p$ | 2.082876 |

### Regressão Simbólica entre os $\Delta x$ e $\Delta p$, como variáveis independentes.

In [94]:

```
from array import array
pr_in=[]
mul=0
co=0
for i in dp:
    mul=dmp[co]*i
    pr_in.append(mul)
    co=co+1
pr_in
l=np.linspace(-20,20,7)
est_gp.fit(desvf,l)
```

```
    |   Population Average    |             Best Individual              |
---- ------------------------- ------------------------------------------ ----------
 Gen   Length          Fitness   Length          Fitness      OOB Fitness  Time Left
   0    14.12          17.3358       61          4.58152          2.20469      2.61m
   1    13.19          12.2287       63          2.01855          16.5301      2.67m
   2    22.91          12.5299       68          1.48236          19.5784      2.70m
   3    45.90          11.1265       67          1.35883          16.5595      2.79m
   4    57.10          8.42914       74           1.2534          16.1118      2.86m
   5    56.64          8.65533      103         0.940835          17.0272      2.81m
   6    55.98          8.42966       74         0.897443          18.0636      2.33m
   7    55.51          8.75305       89         0.915222          18.4083      2.30m
   8    54.16          8.32359       57          0.83206          5.84937      2.04m
   9    54.13          8.69014       59         0.601793          5.16499      1.84m
  10    51.85           8.2424       59         0.601793          5.16499      1.61m
  11    50.01          8.74759       70         0.566704          2.36483      1.44m
  12    48.89          8.13448       63         0.433342          38.7046      1.21m
  13    51.54          7.87202       75         0.439702           1.6471      1.05m
  14    55.80          7.78783       74         0.409549           1.6472     55.09s
  15    62.10          7.10821       63         0.414798          1.55232     47.78s
  16    65.83           8.2369       79         0.343407          1.43067     45.28s
  17    66.11          7.72361       78         0.387547          1.80321     23.63s
  18    64.58          7.55171       78         0.274171          1.35523     13.55s
  19    63.97          7.15509       77         0.328465            1.395      0.00s
```

Processing math: 100%

Out[94]:

SymbolicRegressor

```
sub(sub(sub(mul(neg(div(X0, X0)), add(neg(X1), div(X0, X1))), inv(add(neg
(-0.046), div(-0.094, X1)))), mul(add(neg(div(add(neg(X1), add(neg(X1), ne
g(X1))), X0)), sin(X1)), neg(sin(X1)))), div(sin(sub(sub(sub(mul(neg(div(X
0, X0)), add(neg(sub(X1, -0.041)), div(X0, X1))), inv(add(neg(-0.046), div
(-0.094, X1)))), sin(0.355)), div(sin(div(-0.094, X1)), sub(X1, -0.04
1)))), sub(X1, -0.041)))
```

### Escore:

In [96]:

```python
print('R2:',est_gp.score(desvf,l))
next_e = sympify(str(est_gp._program), locals=converter)
y4=next_e
```

```
R2: 0.9974758366230793
```

### Equação Proposta:

In [98]:

```python
print(y4)
```

```
-X0/X1 + X1 + (sin(X1) + 3*X1/X0)*sin(X1) + sin(X0/X1 - X1 + 0.306590365235784 - sin
(0.094/X1)/(X1 + 0.041) + 1/(0.046 - 0.094/X1))/(X1 + 0.041) - 1/(0.046 - 0.094/X1)
```

### Regressão Simbólica entre os $\Delta x$ e $\Delta p$, como um produto entre ambas.

In [100…

```python
deltax=np.linspace(2.1,2.83,100)
deltap=np.linspace(0.15,0.94,100)
delta_dp=pd.DataFrame()
delta_dp['deltax']=deltax
delta_dp['deltap']=deltap
c=0
mult=[]
for i in deltax:
   j=deltap[c]*i
   mult.append(j)

   c=c+1
c_inf=0
mult_inf=[]
mult_sup=[]
for i in mult:
    if i<0.5:
        mult_inf.append(i)
        c_inf=c_inf+1
    else:
        mult_sup.append(i)
```

In [101…

```python
est_gp.fit(delta_dp,mult)
```

Processing math: 100%

```
     |    Population Average     |             Best Individual              |
---- ------------------------- ------------------------------------------ ----------
 Gen   Length          Fitness   Length          Fitness      OOB Fitness  Time Left
   0    14.12          9.75688        5                0                0      2.60m
```

Out[101…

▾ SymbolicRegressor

mul(neg(X0), neg(X1))

### Escore:

In [103…

```
print('R2:',est_gp.score(delta_dp,mult))
next_e = sympify(str(est_gp._program), locals=converter)
y5=next_e
```

```
R2: 1.0
```

### Equação

In [105…

```
print(y5)
```

```
X0*X1
```

## As Equações Sugeridas:

In [107…

```
print('As Equações Sugeridas:')
print('____________')
print('')
print('I - y1(X0) =', y1)
print('-------')
print('II - y2(X0) =', y2)
print('-------')
print('III - y3(X0,X1,X2) =', y3)
print('-------')
print('IV - y2_arr(X0) = ',y2_arr)
print('-------')
print('V - y4(X0,X1) = ', y4)
print('-------')
print('VI - y5(X0,X1) = ', y5)
print('-------')
```

As Equações Sugeridas:

_____________

```
I - y1(X0) = 0.333/(0.696*X0**2 + 0.812)
-------
II - y2(X0) = -0.517*X0 + sin(X0)
-------
III - y3(X0,X1,X2) = -0.362*X1/(X0*(cos(X2) - 0.198669330795061))
-------
IV - y2_arr(X0) =  sin(cos(sin(X0 - 0.773) + 0.795601620036366)*cos(1/cos(X0))/(0.13
0625639531083 - 2*X0**3))
-------
V - y4(X0,X1) =  -X0/X1 + X1 + (sin(X1) + 3*X1/X0)*sin(X1) + sin(X0/X1 - X1 + 0.3065
90365235784 - sin(0.094/X1)/(X1 + 0.041) + 1/(0.046 - 0.094/X1))/(X1 + 0.041) - 1/
(0.046 - 0.094/X1)
-------
VI - y5(X0,X1) =  X0*X1
-------
```

In [108…

```
print('I - y1(X0) =', end=" ")
y1
```

I - y1(X0) =

Out[108…

$$\frac{0.333}{0.696X_0^2 + 0.812}$$

In [109…

```
y2
```

Out[109…

$$-0.517X_0 + \sin\left(X_0\right)$$

In [110…

```
y3
```

Out[110…

$$-\frac{0.362X_1}{X_0\left(\cos\left(X_2\right) - 0.198669330795061\right)}$$

In [111…

```
y4
```

Out[111…

$$-\frac{X_0}{X_1} + X_1 + \left(\sin\left(X_1\right) + \frac{3X_1}{X_0}\right)\sin\left(X_1\right) + \frac{\sin\left(\frac{X_0}{X_1} - X_1 + 0.306590365235784 - \frac{\sin\left(\frac{0.094}{X_1}\right)}{X_1+0.041} + \frac{1}{0.046-\frac{0.09}{X_1}}\right.}{X_1 + 0.041}$$

In [112…

```
y5
```

Out[112…

$$X_0X_1$$

Processing math: 100%

In [113…

```
X0=1
y2_arr
```

Out[113…

$$\sin\left(\frac{\cos\left(\sin\left(X_0 - 0.773\right) + 0.795601620036366\right)\cos\left(\frac{1}{\cos\left(X_0\right)}\right)}{0.130625639531083 - 2X_0^3}\right)$$

In [ ]:

In [ ]:

In [ ]:

In [ ]:

Processing math: 100%