Box_potential

April 19, 2021

[1]:
```
__author__ = "@Tssp"
__date__   = "15/04/21"
import sympy as sp
from sympy.abc import n, x, a, b
import numpy as np
import matplotlib.pyplot as plt
from method import Chebyshev_Expansion, np_Chebyshev
```

[2]:
```
Vo_sym, k_sym, xi_sym, L_sym, V_plane_sym = sp.symbols('V_0 k \\xi L V_p')
```

[3]:
```
kb = 8.617e-5                # a.u
ao = 5.2917720859e-11        # a.u
Vo = kb * 2e-6               # a.u
V_plane = 0.0 * Vo          # a.u
L = 35e-6/ao                 # a.u
k = 2*np.pi/(532e-9/ao)      # a.u
xi = (Vo + (L/2)**12)**(1/12)# a.u
params = {k_sym: k,
         Vo_sym: Vo,
         xi_sym: xi,
         L_sym: L,
         V_plane_sym: V_plane}
print(f'''
       Parameters
------------------------
Vo[a.u]:       {Vo}
V_plane[a.u]: {V_plane}
L[a.u]:        {L}
wL[nm]:        {532}
k[a.u]:        {k}
xi[a.u]:       {xi}
''')
```

```
       Parameters
------------------------
Vo[a.u]:       1.7234e-10
V_plane[a.u]: 0.0
```

```
L[a.u]:        661404.146509975
wL[nm]:        532
k[a.u]:        0.0006249846732907886
xi[a.u]:       330702.07325498725
```

[4]:
```
V = sp.Piecewise((Vo_sym, x<=-xi_sym), (x**12 + a, x<=-L_sym/2), (0, x<=L_sym/
↪2),\
                 (x**12 + a, x<=xi_sym), (Vo_sym, x>=xi_sym))
V
```

[4]:

$$\begin{cases} V_0 & \text{for}\ \xi \leq -x \\ a + x^{12} & \text{for}\ x \leq -\frac{L}{2} \\ 0 & \text{for}\ x \leq \frac{L}{2} \\ a + x^{12} & \text{for}\ \xi \geq x \\ V_0 & \text{for}\ \xi \leq x \end{cases}$$

Continuity conditions leads to:

$$\xi = (V_0 + (L/2)^{12})^{1/12}$$

$$a = -(L/2)^{12}$$

[5]:
```
V = sp.Piecewise((Vo_sym, x<=-xi_sym), (x**12 - (L_sym/2)**12, x<=-L_sym/2),␣
↪(0, x<=L_sym/2),\
                 (x**12 - (L_sym/2)**12, x<=xi_sym), (Vo_sym, x>=xi_sym))
V = V.subs({xi_sym: (Vo_sym + (L_sym/2)**12)**(1/12)})
V
```

[5]:

$$\begin{cases} V_0 & \text{for}\ x \leq -\left(\frac{L^{12}}{4096} + V_0\right)^{0.0833333333333333} \\ -\frac{L^{12}}{4096} + x^{12} & \text{for}\ x \leq -\frac{L}{2} \\ 0 & \text{for}\ x \leq \frac{L}{2} \\ -\frac{L^{12}}{4096} + x^{12} & \text{for}\ x \leq \left(\frac{L^{12}}{4096} + V_0\right)^{0.0833333333333333} \\ V_0 & \text{for}\ x \geq \left(\frac{L^{12}}{4096} + V_0\right)^{0.0833333333333333} \end{cases}$$

[6]:
```
# Dimensionless
V = V.subs({x: x*(xi_sym + L_sym)})
V
```

[6]:

$$\begin{cases} V_0 & \text{for}\ x\left(L + \xi\right) \leq -\left(\frac{L^{12}}{4096} + V_0\right)^{0.0833333333333333} \\ -\frac{L^{12}}{4096} + x^{12}\left(L + \xi\right)^{12} & \text{for}\ \frac{L}{2} \leq -x\left(L + \xi\right) \\ 0 & \text{for}\ \frac{L}{2} \geq x\left(L + \xi\right) \\ -\frac{L^{12}}{4096} + x^{12}\left(L + \xi\right)^{12} & \text{for}\ x\left(L + \xi\right) \leq \left(\frac{L^{12}}{4096} + V_0\right)^{0.0833333333333333} \\ V_0 & \text{for}\ x\left(L + \xi\right) \geq \left(\frac{L^{12}}{4096} + V_0\right)^{0.0833333333333333} \end{cases}$$

[7]:

```
k_value = 100
Vo_value= 1
L_value = 1
xi_value= (Vo_value + (L_value/2)**12)**(1/12)
params = {k_sym: k_value,
          Vo_sym: Vo_value,
          xi_sym: xi_value,
          L_sym: L_value}
```

[8]:

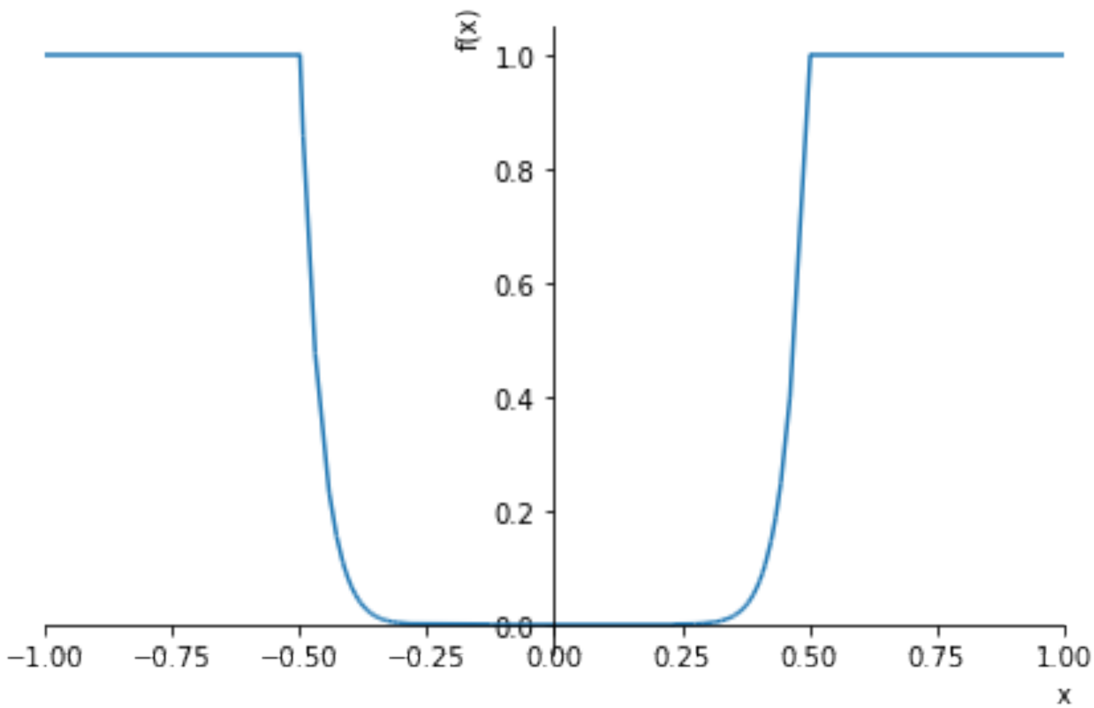
```
V_function = V.subs(params)
V_function
```

[8]:

$$\begin{cases} 1 & \text{for}\ 2.00002034277587x \leq -1.00002034277587 \\ 4096.49997202896x^{12} - \frac{1}{4096} & \text{for}\ 2.00002034277587x \leq -\frac{1}{2} \\ 0 & \text{for}\ 2.00002034277587x \leq \frac{1}{2} \\ 4096.49997202896x^{12} - \frac{1}{4096} & \text{for}\ 2.00002034277587x \leq 1.00002034277587 \\ 1 & \text{for}\ 2.00002034277587x \geq 1.00002034277587 \end{cases}$$

[9]:

```
sp.plotting.plot(V.subs(params), xlim=(-1, 1))
```



[9]: <sympy.plotting.plot.Plot at 0x114809490>