# double_well

August 28, 2019

## 1 Solução/Raízes das Equações Transcendentais

### 1.1 1 Energias abaixo da barreira de potencial

[2]:
```
#libraries

import numpy as np
from scipy import optimize
from scipy.optimize import fsolve
import matplotlib.pyplot as plt
from matplotlib import style
import sympy
from sympy import *
style.use('ggplot')

# Parametros

h_bar = 1
m = 1
V_0 = 50
a = 0.5
L = 1
```

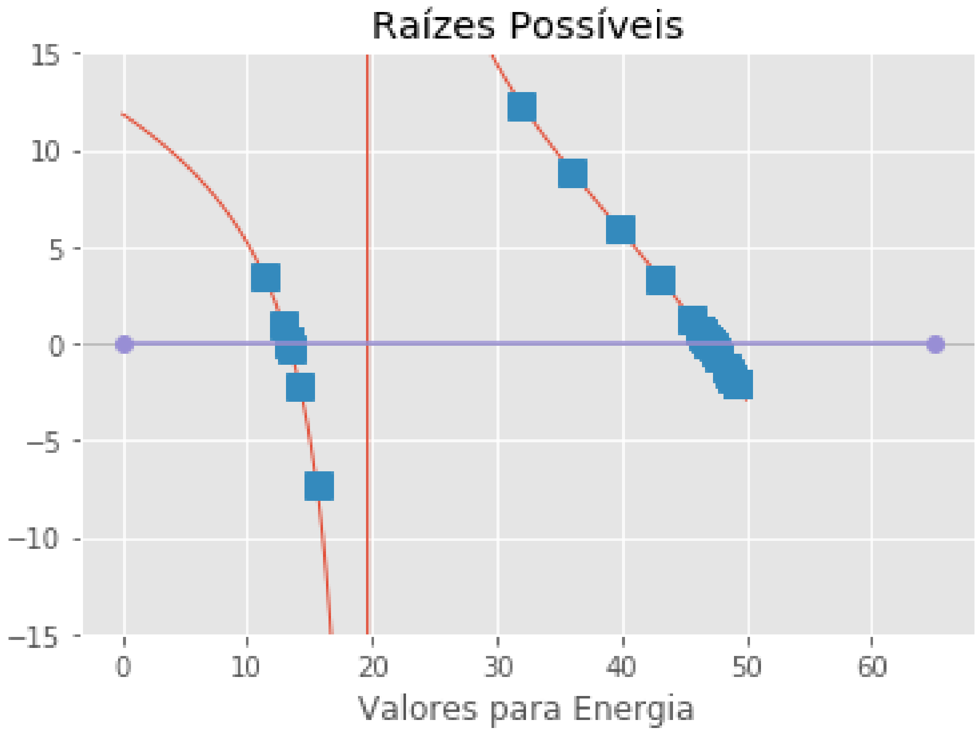
**1.1 E < V_0**

[17]:
```
# Equação #1 de Energia

def func_1(E_1):
    k = np.sqrt(2 * m * E_1) / h_bar # k (região V_0 = 0)
    B = np.sqrt(2 * m * (V_0 - E_1)) / h_bar # B (região V_0 != 0)
    eq1 = k * (1 / np.tan(k * a)) + B * np.tanh(B / 2 * (L - a)) # primeira␣
 ↪equação transcendental (red)
    return eq1

raizes1 = fsolve(func_1, list(range(11,50))) #rotina scipy, 'chutando' um range␣
 ↪de vizinhos próximos das interseções
solucao1 = print(raizes1)
```

```python
# Gráfico das raízes

E_1 = np.linspace(-500,500,10000)
plt.plot(E_1,func_1(E_1),lw=1)
plt.plot(raizes1,func_1(raizes1),'s',ms=10)
plt.axhline(0,color='gray',lw=0.5)
plt.ylim([-15,15])
plt.plot([0,65],[0,0],'o-')
plt.xlabel('Valores para Energia')
plt.title('Raízes Possíveis')
plt.show()
```

```
[11.39613346 12.90375241 13.34913448 13.33435119 13.27909209 13.4956831
 14.21587707 15.59534823 17.70880795 20.54416668 24.00209525 27.90532002
 32.01921999 36.0819951  39.83970509 43.07980392 45.65695709 47.50672578
 48.64549576 49.15791702 49.1755013  48.85138807 48.33642178 47.76060792
 47.22209811 46.78377917 46.47590926 46.30248847 46.24907822 46.29035777
 46.39641677 46.53741907 46.68668905 46.82249281 46.92885029 46.99569137
 47.01860751 46.99838124 46.94041464]
```

```
/home/paulo/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py:5:
RuntimeWarning: invalid value encountered in sqrt
  """
/home/paulo/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py:4:
RuntimeWarning: invalid value encountered in sqrt
  after removing the cwd from sys.path.
```




[23]:
```
# Equação #2 de Energia

def func_2(E_2):
    k = np.sqrt(2 * m * E_2) / h_bar # k (região V_0 = 0)
    B = np.sqrt(2 * m * (V_0 - E_2)) / h_bar # B (região V_0 != 0)
    eq2 = k * (1 / np.tan(k * a)) +  B * (1 / np.tanh(B / 2 * (L - a))) #␣
 ↪segunda equação transcendental (green)
    return eq2

raizes2 = fsolve(func_2, list(range(10,25))) #rotina scipy, 'chutando' vizinhos␣
 ↪próximos da interseção
solucao2 = print(raizes2)

# Gráfico das Soluções
E_2 = np.linspace(-500,500,100000)
plt.plot(E_2,func_2(E_2),lw=1)
plt.plot(raizes2,func_2(raizes2),'s',ms=10)
plt.axhline(0,color='gray',lw=0.5)
plt.ylim([-15,15])
plt.plot([0,60],[0,0],'o-')
plt.xlabel('Valores para Energia')
plt.title('Raízes Possíveis')
plt.show()
```

```
[22.13258047 18.3382158  14.77963507 13.62390267 13.57680593 13.28784337
 12.75715472 12.67300461 13.76353671 16.52085817 21.10721819 27.33732033
 34.71083984 42.49163797 49.82822099]

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  """
```
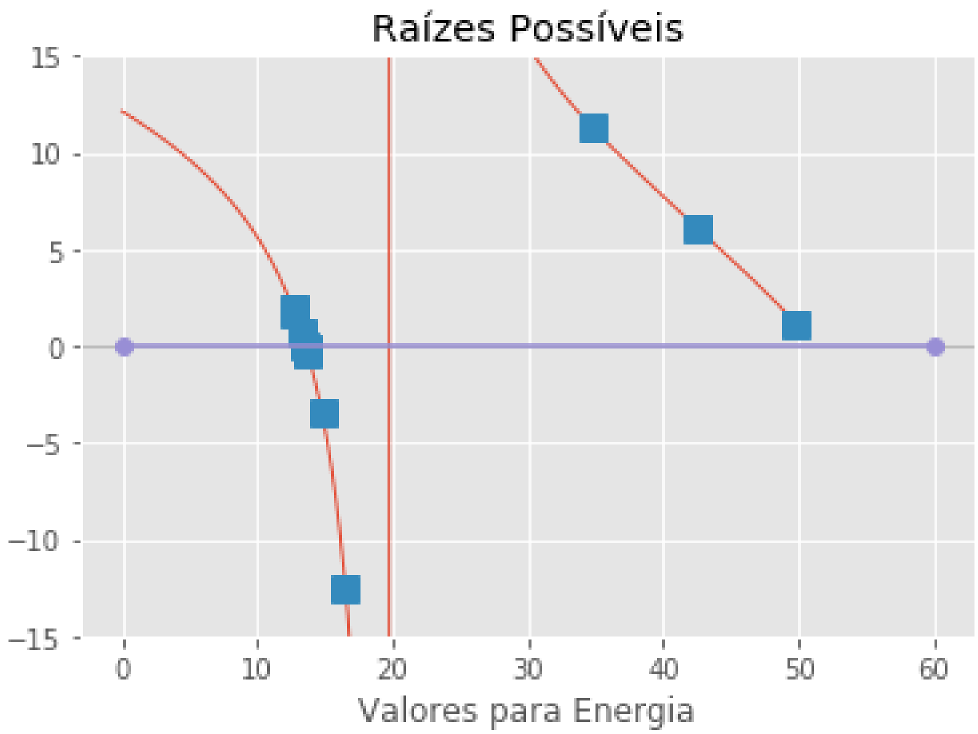




## 1.2 2 Energias acima da barreira de potencial

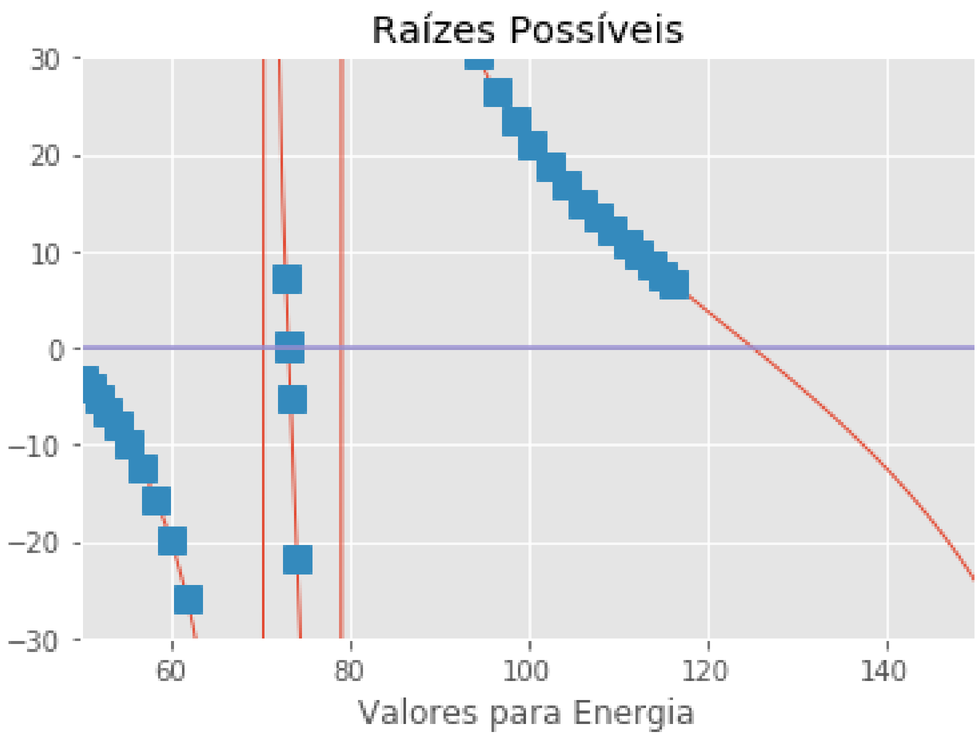
**2.1 E > V_0**

[22]:
```
# Equação #3 de Energia
def func_3(E_3):
    k = np.sqrt(2 * m * E_3) / h_bar # k (região V_0 = 0)
    B = np.sqrt(2 * m * (E_3 - V_0)) / h_bar # B (região E > V_0 !!!)
    eq3 = k * (1 / np.tan(k * a)) -  B * np.tan(B / 2 * (L - a)) # primeira␣
 ↪equação transcendental (red)
    return eq3
```

```
raizes3 = fsolve(func_3,list(range(57, 100))) #rotina scipy, 'chutando'␣
 ↪vizinhos próximos da interseção
solucao3 = print(raizes3)

# Gráfico das Soluções
E_3 = np.linspace(-500,500,1000)
plt.plot(E_3,func_3(E_3),lw=1)
plt.plot(raizes3,func_3(raizes3),'s',ms=10)
plt.axhline(0,color='gray',lw=0.5)
plt.ylim([-30,30])
plt.xlim([50,150])
plt.plot([0,160],[0,0],'o-')
plt.xlabel('Valores para Energia')
plt.title('Raízes Possíveis')
plt.show()
```

```
[ 50.27041738  51.06960526  51.97668441  52.99759722  54.13877681
  55.40725722  56.8106892   58.35708014  60.05384241  61.90522691
  63.90619763  66.02907297  68.19778028  70.24965911  71.91531205
  72.91160741  73.21002325  73.207857    73.44330824  74.19980643
  75.47092038  77.12901357  79.04331292  81.11571244  83.27965635
  85.49084533  87.71912176  89.94301506  92.14640006  94.31652678
  96.44288245  98.51654098 100.52979817 102.47596928 104.34928118
 106.14481307 107.8584654  109.48693937 111.02771756 112.47904426
 113.83989881 115.10996457 116.28959004]
```

```
/home/paulo/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py:4:
RuntimeWarning: invalid value encountered in sqrt
  after removing the cwd from sys.path.
/home/paulo/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py:3:
RuntimeWarning: invalid value encountered in sqrt
  This is separate from the ipykernel package so we can avoid doing imports
until
```




[18]:
```
# Equação #4 de Energia
def func_4(E_4):
    k = np.sqrt(2 * m * E_4) / h_bar # k (região V_0 = 0)
    B = np.sqrt(2 * m * (E_4 - V_0)) / h_bar # B (região E > V_0 !!!)
    eq4 = -k * (1 / np.tan(k * a)) -  B * (1 / np.tan(B / 2 * (L - a))) #␣
↪segunda equação transcendental E > V_0 (green)
    return eq4

raizes4 = fsolve(func_4,list(range(120, 250))) #rotina scipy, 'chutando'␣
↪vizinhos próximos da interseção
solucao4 = print(raizes4)

# Gráfico das Soluções
E_4 = np.linspace(-500,500,1000)
plt.plot(E_4,func_4(E_4),lw=1)
plt.plot(raizes4,func_4(raizes4),'s',ms=10)
plt.axhline(0,color='gray',lw=0.5)
plt.ylim([-1.5,1.5])
plt.xlim([50,250])
plt.plot([0,500],[0,0],'o-')
plt.xlabel('Valores para Energia')
plt.title('Raízes Possíveis')
plt.show()
```

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[100.39073718  51.37521462  51.37521462  51.37521462  51.37521458
 100.39073718 100.39073718 100.39073718 100.39073718 156.20313369
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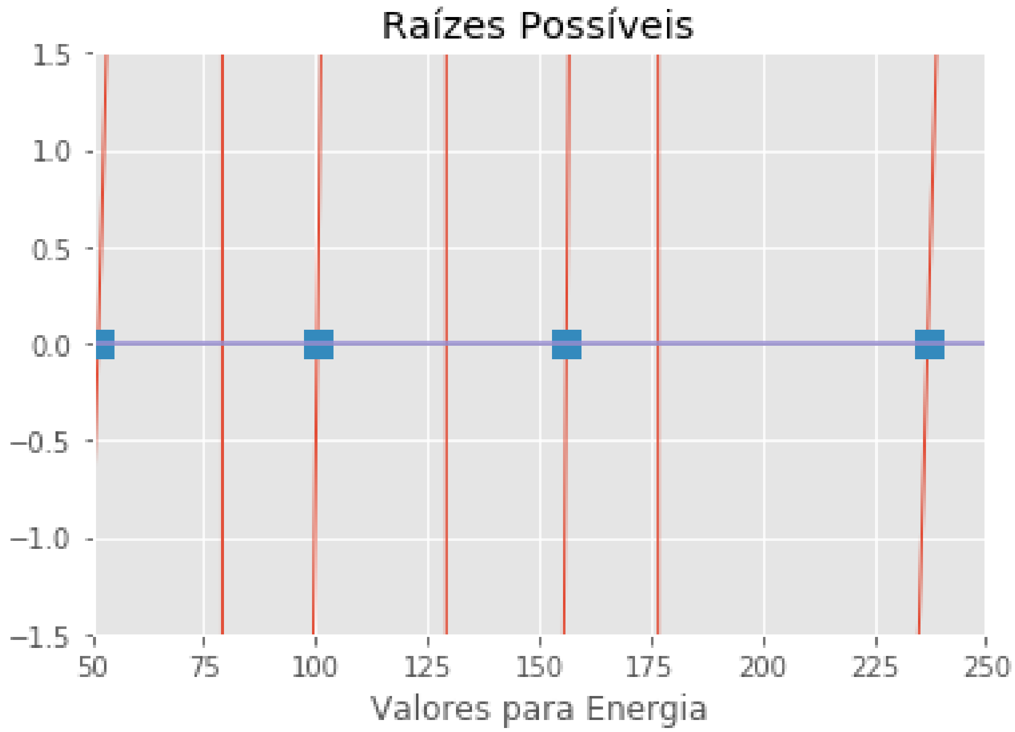
Raízes Possíveis
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
50
75
100
125
150
175
200
225
250
Valores para Energia

[ ]: