

# eigenvalue\_analysis

July 26, 2019

In condensed matter physics, the Su Schrieffer Heeger-modell describes an infinite polyacetylene ( $H_2C_2$ )<sub>n</sub> chain. The Hamiltonian-operator of the model is a 2x2 Hermitian-matrix

$$\begin{pmatrix} 0 & 1 + we^{-ik} \\ 1 + we^{ik} & 0 \end{pmatrix}$$

The wave number  $k$  can vary between  $[-\pi, \pi]$  and  $w$  is a real number between 0.5 and 1.5

The allowed vibrational modes of the molecule are quantised according to QM. These can be determined by finding the eigenvalues of the Hamiltonian with respect to  $k$ .

The parameter  $w$  can be varied manually to see how the eigenvalue distribution changes with different values

```
[9]: %pylab inline
from ipywidgets import *

def abrazil(w):

    k = linspace(-pi, pi, 100) # Values for k in the allowed interval
    lambda_1 = zeros(len(k))   # Vectors for the eigenvalues (2x2
    →Hermitian-matrix has 2 eigenvalues)
    lambda_2 = zeros(len(k))
    for i in range(len(k)):    # We calculate the eigenvalues for each k values
        Hi = matrix([[0, 1 + w * exp(-1j * k[i])], [1 + w * exp(1j * k[i]), 0]])
        lambda_1[i], lambda_2[i] = eig(Hi)[0]
        plot(k, lambda_1)      # We plot the eigenvalues with respect to the
    →wave number k
    plot(k, lambda_2)
    xlabel("k wave number", size=12)
    ylabel("eigenvalue", size=12)
    title("Eigenvalues with respect to wave number", size=18, y = 1.05)
    xticks(linspace(-4, 4, 9))
    yticks(linspace(-3, 3, 7))

    print('The eigenvalues of the Hamiltonian with respect to k, where the value of
    →w can be varied manually')
    interact(abrazil, w=FloatSlider(min=-0.5, max=1.5, step=0.02, value=0.5))
```

Populating the interactive namespace from numpy and matplotlib

The eigenvalues of the Hamiltonian with respect to  $k$ , where the value of  $w$  can be varied manually

```
interactive(children=(FloatSlider(value=0.5, description='w', max=1.5, min=-0.5, step=0.02), Out[9]:
```

```
[9]: <function __main__.abrazol(w)>
```

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[ ]:
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