FYS5419: Project 1

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Imports

In [1]:
```
### Regular imports ###
import numpy as np
import sympy as sp
from time import time
from tqdm import tqdm
from numba import njit
from tabulate import tabulate
import matplotlib.pyplot as plt
from dataclasses import dataclass
from warnings import filterwarnings
from numpy.exceptions import ComplexWarning
from numpy import float64, complex128, ndarray
from typing import Annotated, Literal, Callable

### Customizations ###
np.set_printoptions(precision=3, sign=' ')
%matplotlib inline
plt.rcParams.update({'font.size': 12,
                     'font.family': 'serif',
                     'figure.figsize': (10, 6),
                     'mathtext.fontset': 'cm',
                     'axes.prop_cycle': plt.cycler(color=["#3d0dce",
                                                          "#ff1e1e",
                                                          "#61ffa6",
                                                          "#86db0f",
                                                          "#f711ff",
                                                          "#64B5CD"]),
                     'lines.linewidth': 3,
                     'legend.fontsize': 12,
                    })
tensor_prod = np.kron

### Qiskit imports ###
from qiskit_aer import AerSimulator, Aer
from qiskit.visualization import plot_histogram
```

```
from qiskit.circuit import QuantumCircuit, Parameter
from qiskit_algorithms import VQE, NumPyMinimumEigensolver
from qiskit_algorithms.optimizers import AQGD, COBYLA
from qiskit.quantum_info import SparsePauliOp
from qiskit.primitives import Estimator
```

Types

In [2]:
```
### Matplotlib Figure type ###
Figure = Annotated[plt.Figure, "Figure"]

### Indexing types ###
Indexing_2qbit = Annotated[Literal[0, 1,], "Valid 2 qubit indexing"]
Indexing_3qbit = Annotated[Literal[0, 1, 2], "Valid 3 qubit indexing"]

### Vectors ###
Array2D   = Annotated[ndarray[2, float],   "2D array"]
Array2D_c = Annotated[ndarray[2, complex], "2D complex array"]

Array4D   = Annotated[ndarray[4, float],   "4D array"]
Array4D_c = Annotated[ndarray[4, complex], "4D complex array"]

### Matrices ###
Array2x2   = Annotated[ndarray[(ndarray[2, float],
                                ndarray[2, float])],   "2x2 matrix"]

Array2x2_c = Annotated[ndarray[(ndarray[2, complex],
                                ndarray[2, complex])], "2x2 complex matrix"]

Array4x4   = Annotated[ndarray[(ndarray[4, float],
                                ndarray[4, float])],   "4x4 matrix"]

Array4x4_c = Annotated[ndarray[(ndarray[4, complex],
                                ndarray[4, complex])], "4x4 complex matrix"]

Array5x5  = Annotated[ndarray[(ndarray[5, float],
                               ndarray[5, float])],   "5x5 matrix"]

Array5x5_c = Annotated[ndarray[(ndarray[5, complex],
                                ndarray[5, complex])], "5x5 complex matrix"]
```

a)

Functions

In [3]:
```
@njit
def qubit_basis() -> tuple[Array2D, Array2D]:
    '''
    Creates the qubits standard qubit basis: |0⟩ and |1⟩.
```

```
    Returns
    -------
        q0: Array2D
            |0⟩ = [1, 0]
        q1: Array2D
            |1⟩ = [0, 1]
    '''
    q0: Array2D = np.array([1, 0])
    q1: Array2D = np.array([0, 1])
    return q0, q1

@njit
def pauli() -> tuple[Array2x2_c, Array2x2_c, Array2x2_c]:
    '''
    Creates the Pauli matrices σ_x, σ_y, and σ_z.

    Returns
    -------
        σ_x: Array2x2_c
            Pauli X
        σ_y: Array2x2_c
            Pauli Y
        σ_z: Array2x2_c
            Pauli Z
    '''
    σ_x: Array2x2_c = np.array([[0,  1 ],
                                [1,  0]], dtype=complex128)

    σ_y: Array2x2_c = np.array([[0, -1j],
                                [1j, 0]], dtype=complex128)

    σ_z: Array2x2_c = np.array([[1,  0 ],
                                [0, -1]], dtype=complex128)
    return σ_x, σ_y, σ_z

def hadamard() -> Array2x2:
    '''
    Creates the Hadamard gate.

    Returns
    -------
        H: Array2x2
            Hadamard gate
    '''
    H: Array2x2 = 1/np.sqrt(2) * np.array([[1, 1],
                                           [1, -1]])
    return H

def phase() -> Array2x2_c:
    '''
    Creates the phase gate.

    Returns
    -------
        S: Array2x2_c
            Phase gate
```

```
    '''
    S = np.array([[1,  0],
                  [0, 1j]])
    return S

@njit
def cnot() -> Array4x4_c:
    '''
    Creates the CNOT gate.

    Returns
    -------
        CNOT: Array4x4_c
            CNOT gate
    '''
    CNOT: Array4x4_c = np.array([[1, 0, 0, 0],
                                 [0, 1, 0, 0],
                                 [0, 0, 0, 1],
                                 [0, 0, 1, 0]], dtype=complex128)
    return CNOT

def create_bell_states() -> tuple[Array4D, Array4D, Array4D, Array4D]:
    '''
    Creates the Bell states |Φ⁺⟩, |Φ⁻⟩, |Ψ^+⟩, and |Ψ⁻⟩.

    Returns
    -------
        Φ_00: Array4x4
            |Φ⁺⟩ = (|00⟩ + |11⟩)/√2
        Φ_10: Array4x4
            |Φ⁻⟩ = (|00⟩ - |11⟩)/√2
        Ψ_01: Array4x4
            |Ψ⁺⟩ = (|01⟩ + |10⟩)/√2
        Ψ_11: Array4x4
            |Ψ⁻⟩ = (|01⟩ - |10⟩)/√2
    '''
    q0, q1 = qubit_basis()

    H:    Array2x2 = hadamard()
    CNOT: Array4D_c = cnot()

    q0_H: Array2D = H @ q0
    q1_H: Array2D = H @ q1

    Φ_00: Array4D = CNOT @ tensor_prod(q0_H, q0) # |Φ⁺⟩ = (|00⟩ + |11⟩)/√2
    Φ_10: Array4D = CNOT @ tensor_prod(q1_H, q0) # |Φ⁻⟩ = (|00⟩ - |11⟩)/√2
    Ψ_01: Array4D = CNOT @ tensor_prod(q0_H, q1) # |Ψ⁺⟩ = (|01⟩ + |10⟩)/√2
    Ψ_11: Array4D = CNOT @ tensor_prod(q1_H, q1) # |Ψ⁻⟩ = (|01⟩ - |10⟩)/√2

    return Φ_00, Φ_10, Ψ_01, Ψ_11

def create_system_vectors(n_qubits: int) -> list[ndarray[float64]]:
    """
    Create the system vectors for a given number of qubits.

    Parameters
```

```
    ----------
    n_qubits : int
        The number of qubits in the system.

    Returns
    -------
    system_vectors : list[ndarray[int]]
        A list of system vectors, where each vector represents a possible st
    """
    q0, q1 = qubit_basis()
    system_vectors = []
    for i in range(2**n_qubits):
        binary_str = f'{i:0{n_qubits}b}'
        state = np.array([1])
        for bit in binary_str:
            state = tensor_prod(state, q0 if bit == '0' else q1)
        system_vectors.append(state)

    return system_vectors



def measure_qubit(qubit: Indexing_2qbit, bell_state: Array4D) -> Literal[0,
    '''
    Makes a measurement on a specified cubit in a Bell state

    Parameters
    ----------
        qubit: int
            Which cubit to measure. In a two-qubit state one could pass eith
        bell_state: Array4D
            The state to measure

    Returns
    -------
        state: Literal[0, 1]
            What state the qubit is in. Either 0 or 1
    '''
    if qubit not in [0, 1]:
        raise ValueError(f"Invalid qubit index. Must be either 0 or 1, not {

    n = len(bell_state)
    n_qubits = int(np.log2(n))

    measurement_probabilities = {'0': 0, '1': 0}
    for i in range(n):
        binary_str = f'{i:0{n_qubits}b}'[qubit] # Count in binary, 0-padded
        prob = bell_state[i]
        measurement_probabilities[binary_str] += np.abs(prob)**2

    # Weighted random choice depending on the state
    result = np.random.choice([0, 1], p=[*measurement_probabilities.values()

    return result

def measure_system(bell_state: Array4D) -> Literal['00', '01', '10', '11']:
```

```
    '''
    Makes a measurement on all qubits in a Bell state

    Parameters
    ----------
        bell_state: Array4D
            The state to measure

    Returns
    -------
        state: Literal['00', '01', '10', '11']
            What state the qubits are in. For a two-qubit system, this would
    '''
    measurement_probabilities = {'00': 0, '01': 0, '10': 0, '11': 0}
    for i, bin_str in enumerate(measurement_probabilities.keys()):
        prob = bell_state[i]
        measurement_probabilities[bin_str] += np.abs(prob)**2

    # Weighted random choice depending on the state
    result = np.random.choice(a=[*measurement_probabilities.keys()],
                              p=[*measurement_probabilities.values()])
    return result
```

Playing with Qubits

- The following explores how the qubit states can be combined to form composite states.
- I also explore how their connection to the bit string representation of the state.
- There seems to be a natural connection between the bit string representation and the order of the qubits in the tensor product. This is used to define the order of the qubits in the tensor product.

In [4]:
```
# Checking the states being as expected and their corresponding binary repre
n_qubits = 2
v1, v2, v3, v4 = create_system_vectors(n_qubits)

bin_strs = [f'{i:0{n_qubits}b}' for i in range(2**n_qubits)]

q0, q1 = qubit_basis()

table = tabulate([[bin_strs[0], '|0⟩⊗|0⟩', tensor_prod(q0, q0), v1],
                  [bin_strs[1], '|0⟩⊗|1⟩', tensor_prod(q0, q1), v2],
                  [bin_strs[2], '|1⟩⊗|0⟩', tensor_prod(q1, q0), v3],
                  [bin_strs[3], '|1⟩⊗|1⟩', tensor_prod(q1, q1), v4]],
                 headers  = ['Binary', 'Product', 'Expected', 'Calculated']
                 tablefmt = 'outline',
                 colalign = ['right', 'center', 'center', 'center']
                )
print(table)
```

```
+----------+-----------+---------------+---------------+
|   Binary |  Product  |   Expected    |  Calculated   |
+==========+===========+===============+===============+
|       00 |  |0⟩⊗|0⟩  | [ 1  0  0  0] | [ 1  0  0  0] |
|       01 |  |0⟩⊗|1⟩  | [ 0  1  0  0] | [ 0  1  0  0] |
|       10 |  |1⟩⊗|0⟩  | [ 0  0  1  0] | [ 0  0  1  0] |
|       11 |  |1⟩⊗|1⟩  | [ 0  0  0  1] | [ 0  0  0  1] |
+----------+-----------+---------------+---------------+
```

In [5]:

```
# Checking the states being as expected
n_qubits = 3
v1, v2, v3, v4, v5, v6, v7, v8 = create_system_vectors(n_qubits)

bin_strs = [f'{i:0{n_qubits}b}' for i in range(2**n_qubits)]

q0, q1 = qubit_basis()

table = tabulate([[bin_strs[0], '|0⟩⊗|0⟩⊗|0⟩', tensor_prod(tensor_prod(q0, c
                  [bin_strs[1], '|0⟩⊗|0⟩⊗|1⟩', tensor_prod(tensor_prod(q0, c
                  [bin_strs[2], '|0⟩⊗|1⟩⊗|0⟩', tensor_prod(tensor_prod(q0, c
                  [bin_strs[3], '|0⟩⊗|1⟩⊗|1⟩', tensor_prod(tensor_prod(q0, c
                  [bin_strs[4], '|1⟩⊗|0⟩⊗|0⟩', tensor_prod(tensor_prod(q1, c
                  [bin_strs[5], '|1⟩⊗|0⟩⊗|1⟩', tensor_prod(tensor_prod(q1, c
                  [bin_strs[6], '|1⟩⊗|1⟩⊗|0⟩', tensor_prod(tensor_prod(q1, c
                  [bin_strs[7], '|1⟩⊗|1⟩⊗|1⟩', tensor_prod(tensor_prod(q1, c
                  headers  = ['Binary', 'Product', 'Expected', 'Calculated']
                  tablefmt = 'outline',
                  colalign = ['right', 'center', 'center', 'center']
                 )
print(table)
```

```
+----------+-------------+---------------------------+----------------------
-----+
|   Binary |   Product   |         Expected          |        Calculated
|
+==========+=============+===========================+======================
=====+
|      000 | |0⟩⊗|0⟩⊗|0⟩ | [ 1  0  0  0  0  0  0  0] | [ 1  0  0  0  0  0  0
0] |
|      001 | |0⟩⊗|0⟩⊗|1⟩ | [ 0  1  0  0  0  0  0  0] | [ 0  1  0  0  0  0  0
0] |
|      010 | |0⟩⊗|1⟩⊗|0⟩ | [ 0  0  1  0  0  0  0  0] | [ 0  0  1  0  0  0  0
0] |
|      011 | |0⟩⊗|1⟩⊗|1⟩ | [ 0  0  0  1  0  0  0  0] | [ 0  0  0  1  0  0  0
0] |
|      100 | |1⟩⊗|0⟩⊗|0⟩ | [ 0  0  0  0  1  0  0  0] | [ 0  0  0  0  1  0  0
0] |
|      101 | |1⟩⊗|0⟩⊗|1⟩ | [ 0  0  0  0  0  1  0  0] | [ 0  0  0  0  0  1  0
0] |
|      110 | |1⟩⊗|1⟩⊗|0⟩ | [ 0  0  0  0  0  0  1  0] | [ 0  0  0  0  0  0  1
0] |
|      111 | |1⟩⊗|1⟩⊗|1⟩ | [ 0  0  0  0  0  0  0  1] | [ 0  0  0  0  0  0  0
1] |
+----------+-------------+---------------------------+----------------------
-----+
```

Exploring Pauli Matrices

In [6]:
```
q0, q1 = qubit_basis()
σ_x, σ_y, σ_z = pauli()

q0_x: Array2D_c = σ_x @ q0
q0_y: Array2D_c = σ_y @ q0
q0_z: Array2D_c = σ_z @ q0

q1_x: Array2D_c = σ_x @ q1
q1_y: Array2D_c = σ_y @ q1
q1_z: Array2D_c = σ_z @ q1

print(f'σ_x|0⟩ = {q0_x}')
print(f'σ_y|0⟩ = {q0_y}')
print(f'σ_z|0⟩ = {q0_z}')
print()
print(f'σ_x|1⟩ = {q1_x}')
print(f'σ_y|1⟩ = {q1_y}')
print(f'σ_z|1⟩ = {q1_z}')
```

```
σ_x|0⟩ = [ 0.+0.j  1.+0.j]
σ_y|0⟩ = [ 0.+0.j  0.+1.j]
σ_z|0⟩ = [ 1.+0.j  0.+0.j]

σ_x|1⟩ = [ 1.+0.j  0.+0.j]
σ_y|1⟩ = [ 0.-1.j  0.+0.j]
σ_z|1⟩ = [ 0.+0.j -1.+0.j]
```

Exploring Gates

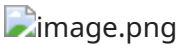
In [7]:
```
H: Array2x2   = hadamard()
S: Array2x2_c = phase()

q0_H = H @ q0
q0_S = S @ q0

q1_H = H @ q1
q1_S = S @ q1

print(f'H|0⟩ = {q0_H}')
print(f'S|0⟩ = {q0_S}')
print()
print(f'H|1⟩ = {q1_H}')
print(f'S|1⟩ = {q1_S}')
```

```
H|0⟩ = [ 0.707  0.707]
S|0⟩ = [ 1.+0.j  0.+0.j]

H|1⟩ = [ 0.707 -0.707]
S|1⟩ = [ 0.+0.j  0.+1.j]
```

Bell States

Example of a Bell State and how to create it using a circuit. In this case, the Bell State $|\Phi^+\rangle$ is created using a Hadamard gate and a CNOT gate:

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\Big(|00\rangle + |11\rangle\Big)$$



Creation by Applying Gates

In [8]:
```
Φ_00, Φ_10, Ψ_01, Ψ_11 = create_bell_states()

print(f'|Φ⁺⟩ = {Φ_00}')
print(f'|Φ⁺⟩ = {Φ_10}')
print(f'|Ψ⁺⟩ = {Ψ_01}')
print(f'|Ψ⁺⟩ = {Ψ_11}')
```

```
|Φ⁺⟩ = [ 0.707+0.j  0.   +0.j  0.   +0.j  0.707+0.j]
|Φ⁺⟩ = [ 0.707+0.j  0.   +0.j  0.   +0.j -0.707+0.j]
|Ψ⁺⟩ = [ 0.   +0.j  0.707+0.j  0.707+0.j  0.   +0.j]
|Ψ⁺⟩ = [ 0.   +0.j  0.707+0.j -0.707+0.j  0.   +0.j]
```

Direct Creation

In [9]:
```
q_00, q_01, q_10, q_11 = create_system_vectors(2)

Φ_00 = 1/np.sqrt(2) * (q_00 + q_11)
Φ_10 = 1/np.sqrt(2) * (q_00 - q_11)
Ψ_01 = 1/np.sqrt(2) * (q_01 + q_10)
Ψ_11 = 1/np.sqrt(2) * (q_01 - q_10)

print(f'|Φ⁺⟩ = {Φ_00}')
print(f'|Φ⁻⟩ = {Φ_10}')
print(f'|Ψ⁺⟩ = {Ψ_01}')
print(f'|Ψ⁻⟩ = {Ψ_11}')
```

```
|Φ⁺⟩ = [ 0.707  0.     0.     0.707]
|Φ⁻⟩ = [ 0.707  0.     0.    -0.707]
|Ψ⁺⟩ = [ 0.     0.707  0.707  0.   ]
|Ψ⁻⟩ = [ 0.     0.707 -0.707  0.   ]
```

Acting on the Bell State with Gates

In [10]:
```
H = hadamard()
CNOT = cnot()
I_2 = np.eye(2)

# Applying the Hadamard and CNOT gate to the first Bell state
Φ_00_H = tensor_prod(H, I_2) @ Φ_00
```

```
Φ_00_H_CNOT = CNOT @ Φ_00_H

print(f'|Φ⁺⟩ =          {Φ_00}')
print(f'(H⊗I)|Φ⁺⟩ =     {Φ_00_H}')
print(f'CNOT(H⊗I)|Φ⁺⟩ = {Φ_00_H_CNOT}')
```

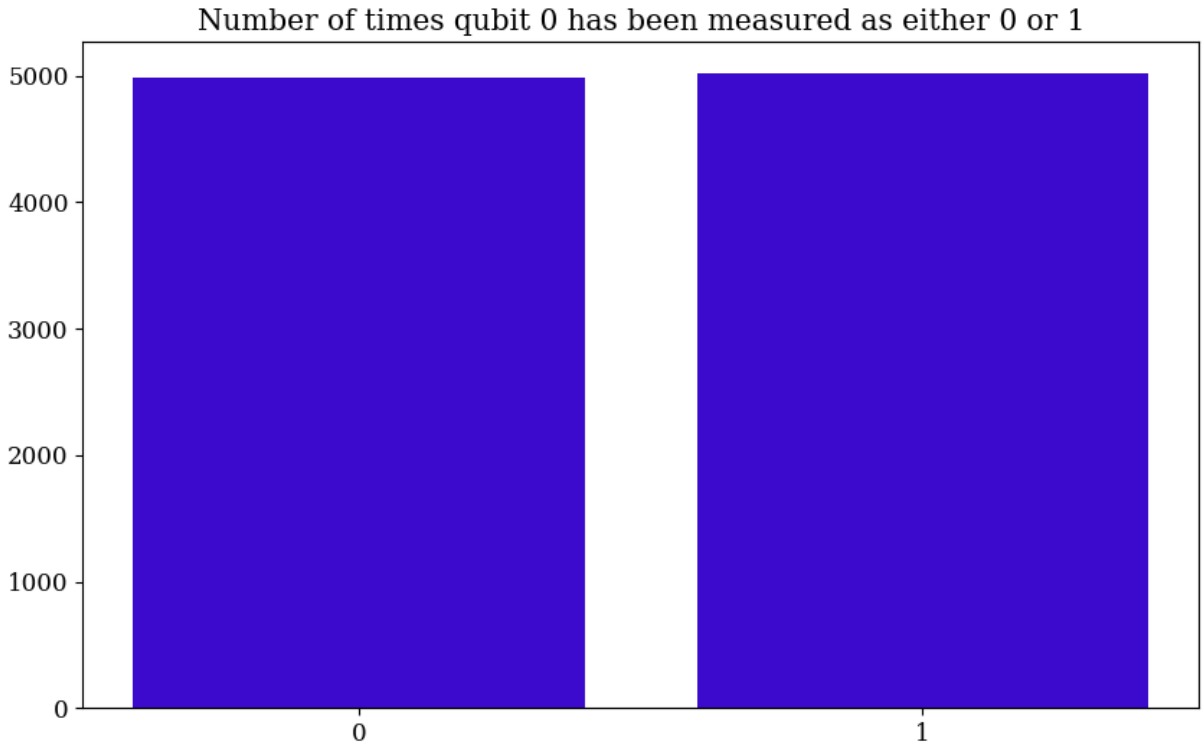
```
|Φ⁺⟩ =          [ 0.707  0.     0.     0.707]
(H⊗I)|Φ⁺⟩ =     [ 0.5  0.5  0.5 -0.5]
CNOT(H⊗I)|Φ⁺⟩ = [ 0.5+0.j  0.5+0.j -0.5+0.j  0.5+0.j]
```

Testing by Measuring Bell States

In [11]:
```
# Making a measurment
q0_results = {0: 0, 1: 0}
q1_results = {0: 0, 1: 0}
n_lambdas = 10_000
for i in range(n_lambdas):
    q0_res = measure_qubit(0, Φ_00)
    q0_results[q0_res] += 1

    q1_res = measure_qubit(1, Φ_00)
    q1_results[q1_res] += 1
```

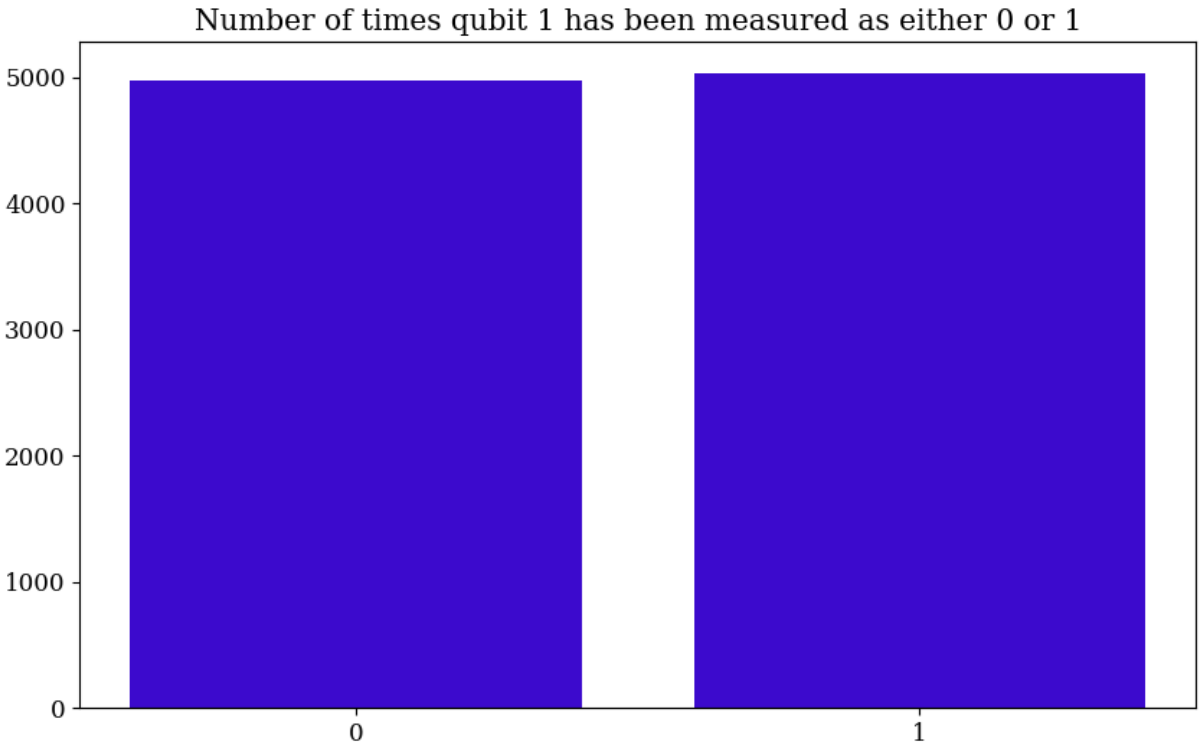
In [12]:
```
print(f'Odds of measuring qubit 0 as 0:, {q0_results[0]/n_lambdas: .2%}')
print(f'Odds of measuring qubit 0 as 1:, {q0_results[1]/n_lambdas: .2%}')

plt.bar(q0_results.keys(), q0_results.values())
plt.xticks([0, 1])
plt.title("Number of times qubit 0 has been measured as either 0 or 1")
plt.savefig('figs/a_q0_measurement.pdf')
plt.show()
```

```
Odds of measuring qubit 0 as 0:,  49.83%
Odds of measuring qubit 0 as 1:,  50.17%
```



In [13]:
```
print(f'Odds of measuring qubit 0 as 0:, {q1_results[0]/n_lambdas: .2%}')
print(f'Odds of measuring qubit 0 as 1:, {q1_results[1]/n_lambdas: .2%}')

plt.bar(q1_results.keys(), q1_results.values())
plt.xticks([0, 1])
plt.title("Number of times qubit 1 has been measured as either 0 or 1")
plt.savefig('figs/a_q1_measurement.pdf')
plt.show()
```

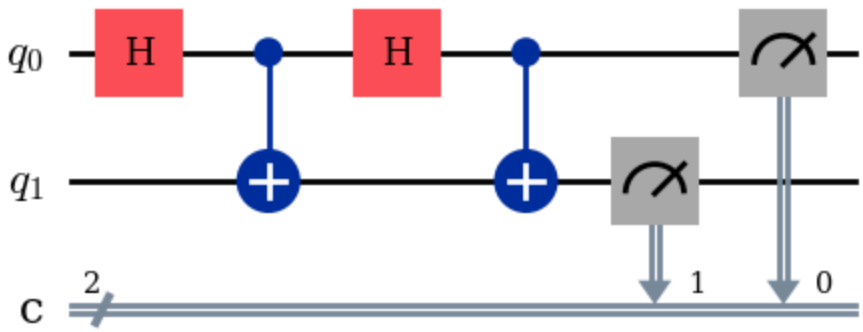
```
Odds of measuring qubit 0 as 0:,  49.74%
Odds of measuring qubit 0 as 1:,  50.26%
```



Circuit and Measurements in Qiskit

In [14]:
```
qc = QuantumCircuit(2, 2)
qc.h(0)
qc.cx(0, 1)
qc.h(0)
qc.cx(0, 1)

# Measureing the qubits
qc.measure(1, 1)
qc.measure(0, 0)
# Needed for qiskit drawing
%matplotlib notebook
qc.draw('mpl')
```

Out[14]:

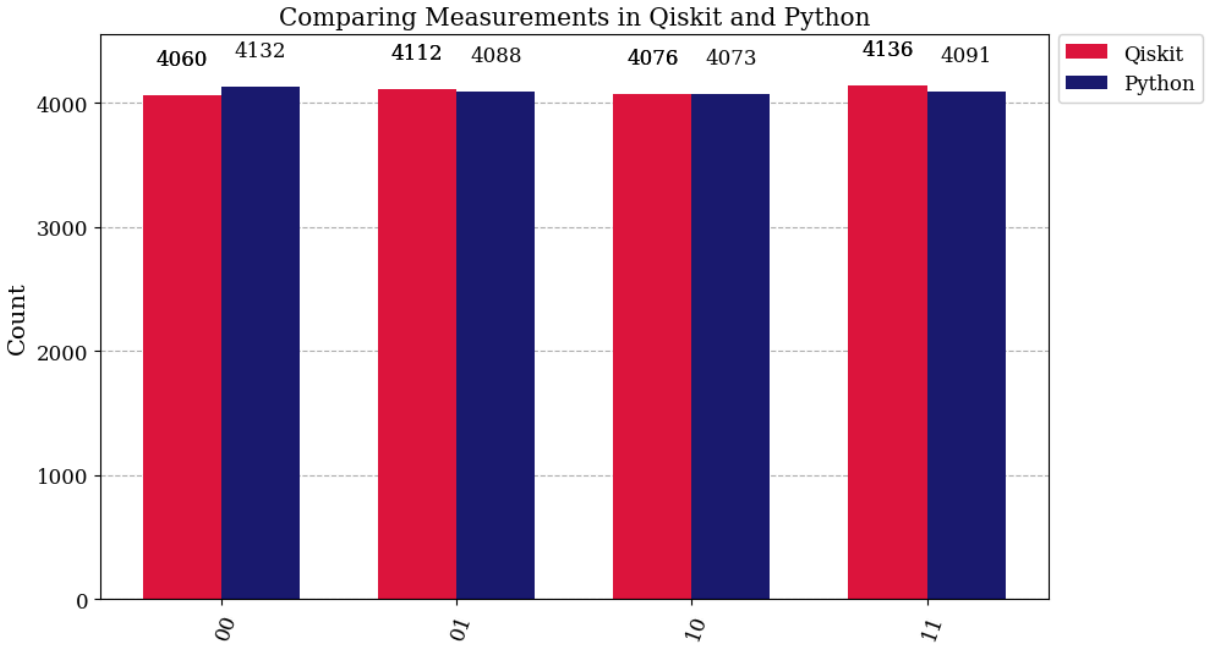


In [15]:
```
# Makes the plots static again after the qiskit drawing
%matplotlib inline
```

Comparing Probabilities from Measurements

In [16]:
```
simulator = AerSimulator()
n_lambdas = 2**14
results_qk = simulator.run(qc, shots=n_lambdas).result().get_counts(qc)
results_qk = dict(sorted(results_qk.items(), key=lambda x: x[0])) # Sort the

# Extracting the probabilities
prob_qk = {key: val/n_lambdas for key, val in results_qk.items()}

# Comparing with python implementation
H = hadamard()
CNOT = cnot()
Φ_00 = create_bell_states()[0]

state = CNOT @ tensor_prod(H, I_2) @ Φ_00

results_py = {f'{i:02b}': 0 for i in range(4)}
for i in range(n_lambdas):
    res = measure_system(state)
    results_py[res] += 1

# Extracting the probabilities
prob_py = {key: val/n_lambdas for key, val in results_py.items()}

table = tabulate([["|00⟩", f'{prob_qk['00']: .2%}', f'{prob_py["00"]: .2%}']
                  ["|01⟩", f'{prob_qk['01']: .2%}', f'{prob_py["01"]: .2%}']
                  ["|10⟩", f'{prob_qk['10']: .2%}', f'{prob_py["10"]: .2%}']
                  ["|11⟩", f'{prob_qk['11']: .2%}', f'{prob_py["11"]: .2%}']
                  headers  = ['State', 'Qiskit', 'Python'],
                  tablefmt = 'outline',
                  colalign = ['center', 'center', 'center']
                 )
print("Probabilities of measuring the Bell states in Qiskit and Python")
print("-----------------------------------------------------------------")
print(table)


fig = plot_histogram([results_qk, results_py], title="Comparing Measurements
                     legend=['Qiskit', 'Python'], color=['crimson', 'midnigh

fig.savefig('figs/a_qiskit_vs_python.pdf')
fig.savefig('selected_results/a_qiskit_vs_python.pdf')
plt.show()
```

```
Probabilities of measuring the Bell states in Qiskit and Python
-----------------------------------------------------------------
+---------+----------+----------+
|  State  |  Qiskit  |  Python  |
+=========+==========+==========+
|  |00⟩   |  24.78%  |  25.22%  |
|  |01⟩   |  25.10%  |  24.95%  |
|  |10⟩   |  24.88%  |  24.86%  |
|  |11⟩   |  25.24%  |  24.97%  |
+---------+----------+----------+
```



Conclusion

- As we can see, the qubit states can be combined to form composite states using the tensor product of $|0\rangle$ and $|1\rangle$.
- We looked at the bell state $|\Phi^+\rangle$, in which both qubits are either in the state $|0\rangle$, represented by $|00\rangle$, or $|1\rangle$ represented by $|11\rangle$.
- Applying a Hadamard and CNOT gate to $|\Phi^+\rangle$, we get the expected results of approximately a 25% chance of measuring either $|00\rangle$, $|01\rangle$, $|10\rangle$ or $|11\rangle$.

b)

Functions

In [17]:
```
@njit
def Hamiltonian_1qbit(λ: float) -> Array2x2_c:
    '''
    Creates the Hamiltonian for a given interaction strength λ.

    Parameters
```

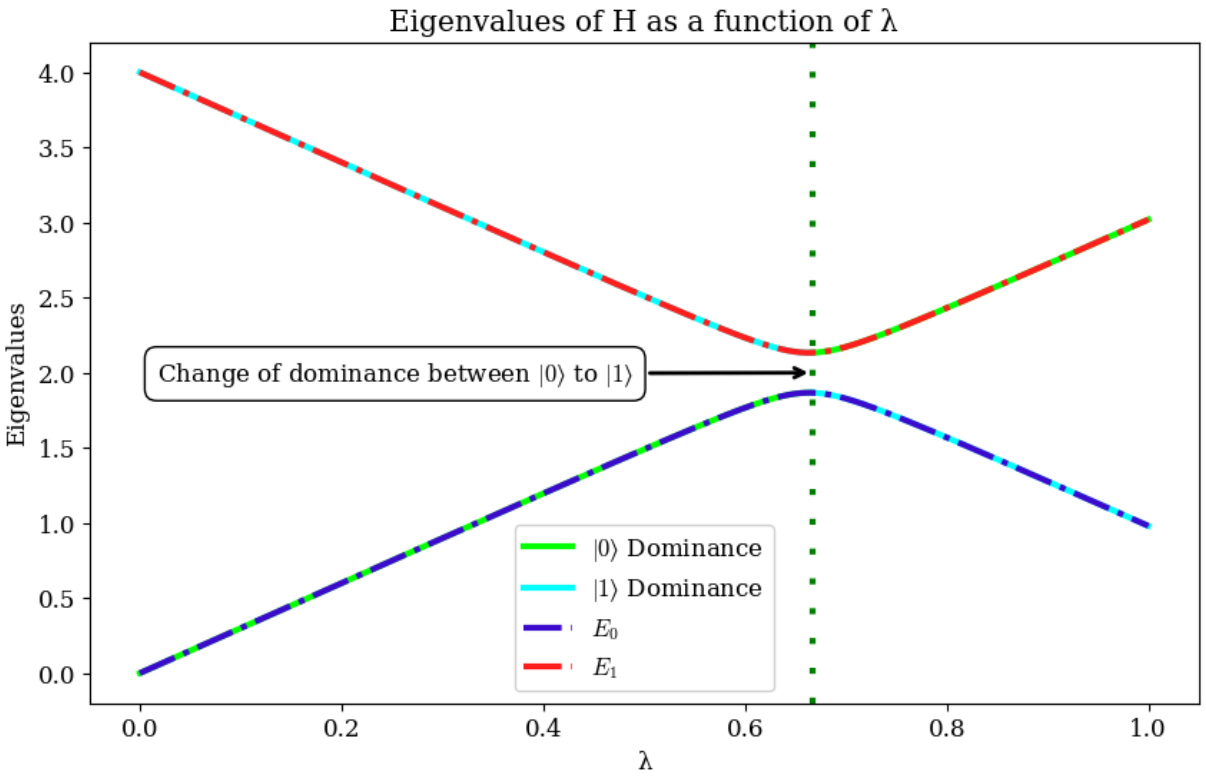
```
    ----------
        λ: float
            The interaction strength

    Returns
    -------
        H: Array2x2_c
            The complex 2x2 Hamiltonian matrix
    '''

    E1 = 0
    E2 = 4
    E = (E1 + E2) / 2
    Ω = (E1 - E2) / 2
    σ_x, σ_y, σ_z = pauli()
    I_2 = np.eye(2, dtype=complex128)
    H0 = E*I_2 + Ω*σ_z

    V11 = 3
    V22 = -V11
    V12 = V21 = 0.2
    c = (V11 + V22) / 2
    ω_z = (V11 - V22) / 2
    ω_x = V12
    HI = c*I_2 + ω_z*σ_z + ω_x*σ_x

    H = H0 + λ*HI
    return H
```

Finding Eigenvalues

In [18]:

```
n_lambdas = 10001
lambdas = np.linspace(0, 1, n_lambdas)
energy_eigvals = [np.linalg.eigvalsh(Hamiltonian_1qbit(λ)).real for λ in lam
E_0, E_1 = np.array(energy_eigvals).T

switch_value = lambdas < 2/3

# Plotting energy eigenstate 0's energy
plt.plot(lambdas[switch_value],  E_0[switch_value], label=r'$|0⟩$ Dominance'
plt.plot(lambdas[~switch_value], E_1[~switch_value], color='lime')

# Plotting energy eigenstate 1's energy
plt.plot(lambdas[switch_value],  E_1[switch_value], label=r'$|1⟩$ Dominance'
plt.plot(lambdas[~switch_value], E_0[~switch_value], color='aqua')

# Plotting the eigenvalues
plt.plot(lambdas, energy_eigvals, label=(r'$E_0$', r'$E_1$'), linestyle='-.'

x = 2/3
y = (energy_eigvals[int(2/3*n_lambdas)][0] + energy_eigvals[int(2/3*n_lambda
plt.annotate(text=r"Change of dominance between $|0⟩$ to $|1⟩$",
             xy=(x, y),
             xytext=(x-.65, y-.05),
```

```
            arrowprops=dict(arrowstyle='->', lw=2),
            bbox=dict(facecolor='white',
            edgecolor='black',
            boxstyle='round,pad=0.5')),

plt.axvline(x=2/3, color='green', linestyle=(0, (1, 4))) # Marking the chang
plt.xlabel('λ')
plt.ylabel('Eigenvalues')
plt.title('Eigenvalues of H as a function of λ')
plt.legend()
plt.savefig('figs/b_eigenvalues.pdf')
plt.savefig('selected_results/b_eigenvalues.pdf')
plt.show()
```



Conclusion

- As the interacting term λ increases, the first energy eigenstate increases in energy, while the second energy eigenstate decreases in energy. They soon after diverge at $\lambda = 2/3$.
- At $\lambda = 2/3$, we see a switch in dominance between which part of our basis is the largest contributor to the energy eigenstates.

c)

Functions

In [19]:

```
@njit
def Rx(θ: float) -> Array2x2_c:
    '''
    Rotation around the x-axis

    Parameters
    ----------
        θ: float
            The angle (radians) to rotate by

    Returns
    -------
        Rx: Array2x2_c
            The complex 2x2 rotation matrix
    '''
    I_2 = np.eye(2)
    X = np.array([[0, 1], [1, 0]], dtype=complex128)
    return np.cos(θ*0.5) * I_2-1j * np.sin(θ*0.5) * X

@njit
def Ry(ϕ: float) -> Array2x2_c:
    '''
    Rotation around the y-axisChange of groundstate bewteen energy eigenstat

    Parameters
    ----------
        ϕ: float
            The angle (radians) to rotate by

    Returns
    -------
        Ry: Array2x2_c
            The complex 2x2 rotation matrix
    '''
    I_2 = np.eye(2)
    Y = np.array([[0, -1j], [1j, 0]])
    return np.cos(ϕ*0.5) * I_2-1j * np.sin(ϕ*0.5) * Y

@njit
def Energy_1qbit(θ: float, ϕ: float, λ: float) -> float:
    '''
    Calculates the energy eigenvalues of the Hamiltonian for a 1-qubit syste

    Parameters
    ----------
        θ: float
            The angle (radians) to rotate by around the x-axis
        ϕ: float
            The angle (radians) to rotate by around the y-axis
        λ: float
            The interaction strength

    Returns
    -------
        E: float
```

```
            The energy eigenvalue (real)
    '''
    q0, q1 = qubit_basis()
    q0: Array2D_c = q0.astype(complex128) # Promoted to complex for njit

    basis = q0 # |0⟩: Will be rotated anyways so no need to use |1⟩
    rotated_basis = Rx(θ) @ Ry(ϕ) @ basis
    E = rotated_basis.conj().T @ Hamiltonian_1qbit(λ) @ rotated_basis

    assert abs(E.imag) < 1e-14, f'Energy is complex. Something went wrong: E
    return E.real

@njit
def VQE_1qbit(n_iterations: int, η: float, λ: float = 0, seed: int = 2024) -
    '''
    Variational Quantum Eigensolver using Gradient Descent to find the minim

    Parameters
    ----------
        N_iterations: int
            Number of iterations
        η: float
            Learning rate
        λ: float
            Interaction strength of the Hamiltonian
        seed: int
            Seed for the random number generator

    Returns
    -------
        Energy(θ, ϕ, λ): float
            The lowest energy eigenvalue found in n iterations (real)
    '''
    π = np.pi
    np.random.seed(seed)
    θ = 2*π*np.random.rand()
    ϕ = 2*π*np.random.rand()
    for _ in range(n_iterations):
        ΔE_Δθ = (Energy_1qbit(θ+π/2, ϕ, λ) - Energy_1qbit(θ-π/2, ϕ, λ)) / 2
        ΔE_Δϕ = (Energy_1qbit(θ, ϕ+π/2, λ) - Energy_1qbit(θ, ϕ-π/2, λ)) / 2
        θ -= η * ΔE_Δθ
        ϕ -= η * ΔE_Δϕ

    E = Energy_1qbit(θ, ϕ, λ)
    return E

@dataclass
class Benchmark_Results():
    '''
    Dataclass for the benchmark results

    Parameters
    ----------
        eig_vals_vqe: ndarray
            The energy eigenvalues found by the VQE algorithm
        eig_vals_numpy: ndarray
```

```
            The energy eigenvalues found by numpy
        lambdas: ndarray
            Interaction strengths
        alg_name: str
            The name of the VQE algorithm
        switch_point: float (optional) = None
            The interaction strength where the groundstate changes
    '''
    eig_vals_vqe: ndarray
    eig_vals_np:  ndarray
    lambdas:      ndarray
    alg_name:     str
    switch_point: float = None


def benchmark_VQE(VQE_alg: Callable, Hamiltonian: Callable, n_iterations: ir
    '''
    Benchmarks a VQE algorithm for a given number of iterations and learning

    Parameters
    ----------
        VQE_alg: Callable
            The VQE algorithm to benchmark
        Hamiltonian: Callable
            The Hamiltonian to pass to numpy
        n_iterations: int
            Number of iterations
        η: float
            Learning rate
        lambdas: ndarray
            Interaction strengths to benchmark

    Returns
    -------
        result: Benchmark_Results
            The benchmark results stored in a dataclass
    '''

    start = time()
    eig_vals_vqe = np.array([VQE_alg(n_iterations, η, λ) for λ in lambdas])
    vqe_time_cold = time() - start

    start = time()
    eig_vals_vqe = np.array([VQE_alg(n_iterations, η, λ) for λ in lambdas])
    vqe_time_warm = time() - start

    start = time()
    eig_vals_numpy = [np.min(np.linalg.eigvals(Hamiltonian(λ))).real for λ i
    numpy_time = time() - start

    name = VQE_alg.__name__
    table = [["Method", "Time (s)", "Times Slower than Numpy"],
             [f"{name} (cold)", f"{vqe_time_cold:.2g}", f"{vqe_time_cold/num
             [f"{name} (warm)", f"{vqe_time_warm:.2g}", f"{vqe_time_warm/num
             ["Numpy", f"{numpy_time:.2g}", "1.00"]
    ]
```

```
    print(tabulate(table, headers="firstrow", tablefmt="grid"))

    result: Benchmark_Results = Benchmark_Results(eig_vals_vqe, eig_vals_num
    return result


def plot_relative_error(result: Benchmark_Results) -> Figure:
    '''
    Plots a comparison between the VQE algorithm and numpy and prints a nice

    Parameters
    ----------
        result: Benchmark_Results
            The benchmark results stored in dataclass

    Returns
    -------
        fig: Figure
            The matplotlib figure (`plt.show()` will be called)
    '''
    eig_vals_vqe = result.eig_vals_vqe
    eig_vals_numpy = result.eig_vals_np
    lambdas = result.lambdas

    filterwarnings("ignore", category=RuntimeWarning) # Ignore RuntimeWarnir
    relative_error = np.abs(eig_vals_vqe - eig_vals_numpy) / np.abs(eig_vals
    filterwarnings("default", category=RuntimeWarning) # Turn warning back o

    plt.plot(lambdas, relative_error, label=f'Relative error')

    switch_point = result.switch_point
    plt.axvline(x=switch_point, color='green', linestyle=(0, (1, 5)), label=

    width = 1/15
    plt.axvspan(switch_point - width, switch_point + width , color='red', al

    zeros = np.where(relative_error == 0)[0]
    if len(zeros) > 0:
        plt.scatter(lambdas[zeros], relative_error[zeros], color='black', la

    plt.xlabel('λ')
    plt.ylabel('Relative error')

    percentage_formatter = lambda x, _: f'{x*100:1g}%'
    plt.gca().yaxis.set_major_formatter(plt.FuncFormatter(percentage_formatt
    plt.legend()

    return plt.gcf()

def plot_eigvals(result: Benchmark_Results) -> Figure:
    '''
    Plots a comparison between the VQE algorithm and numpy

    Parameters
    ----------
        result: Benchmark_Results
```

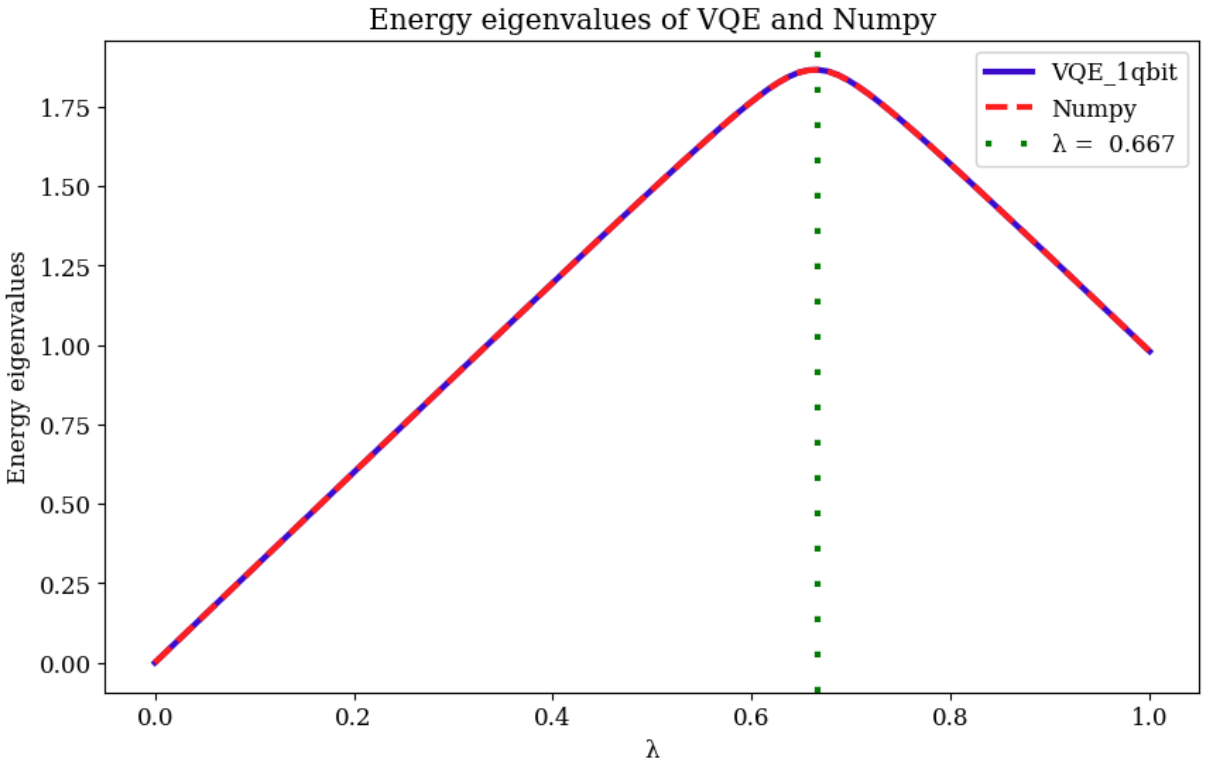
```
            The benchmark results stored in a named tuple
    '''
    eig_vals_vqe = result.eig_vals_vqe
    eig_vals_numpy = result.eig_vals_np
    lambdas = result.lambdas
    switch_point = result.switch_point
    alg_name = result.alg_name

    plt.plot(lambdas, eig_vals_vqe, label=f'{alg_name}')
    plt.plot(lambdas, eig_vals_numpy, label='Numpy', linestyle='--')

    plt.axvline(x=switch_point, color='green', linestyle=(0, (1, 5)), label=
    plt.xlabel('λ')
    plt.ylabel('Energy eigenvalues')
    plt.legend()

    return plt.gcf()

def error_statistics(result: Benchmark_Results) -> None:
    '''
    Prints out statistics for the benchmark results

    Parameters
    ----------
        result: Benchmark_Results
            The benchmark results stored in a named tuple
    '''
    eig_vals_vqe = result.eig_vals_vqe
    eig_vals_numpy = result.eig_vals_np

    filterwarnings("ignore", category=RuntimeWarning) # Ignore RuntimeWarnir
    relative_error = np.abs(eig_vals_vqe - eig_vals_numpy) / np.abs(eig_vals
    filterwarnings("default", category=RuntimeWarning) # Turn warning back o

    # Remove infinites after division by zero
    non_inf = np.isfinite(relative_error)
    relative_error = relative_error[non_inf]

    mean_error   = np.mean(relative_error)
    median_error = np.median(relative_error)
    max_error    = np.max(relative_error)
    min_error    = np.min(relative_error)
    std_error    = np.std(relative_error)

    table = [["Mean",   f'{mean_error*100: .1g}%'],
             ["Median", f'{median_error*100: .1g}%'],
             ["Max",    f'{max_error*100: .1g}%'],
             ["Min",    f'{min_error*100: .1g}%'],
             ["Std",   f'{std_error*100: .1g}%']]
    print(tabulate(table, headers=['Metric', 'Error (%)'], tablefmt="outline
```

Comparing VQE and Exact Eigenvalues

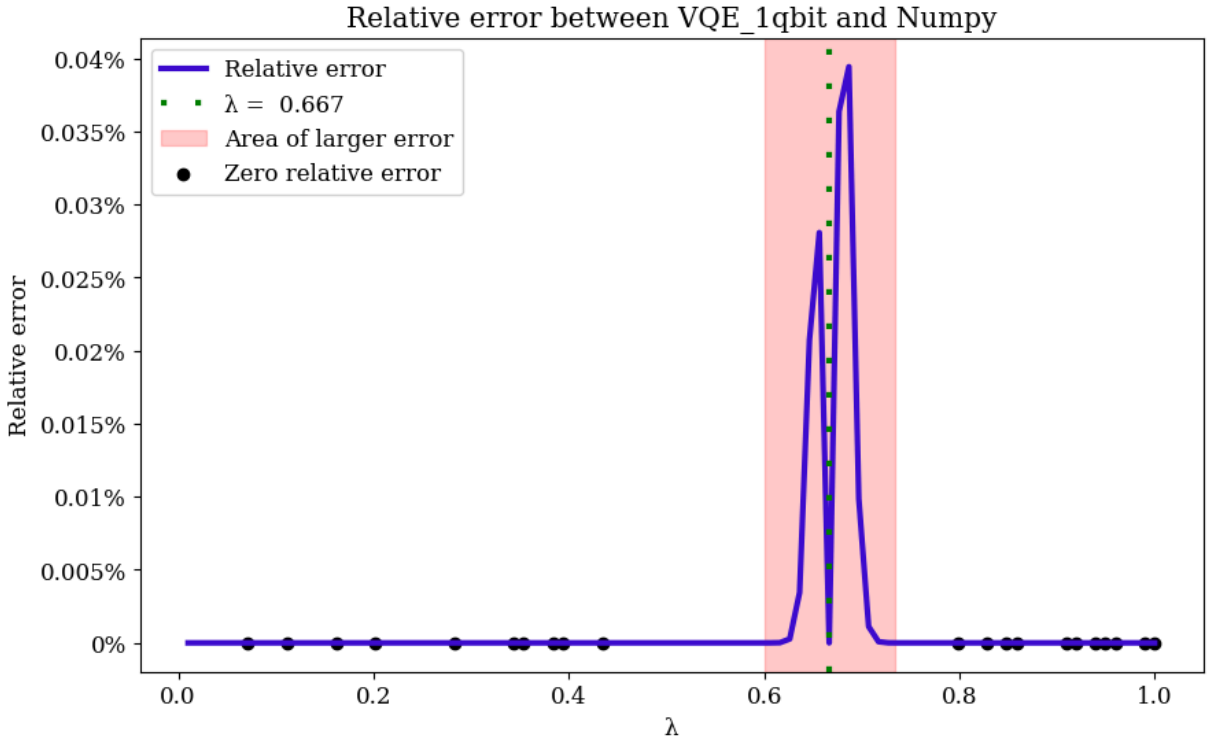
In [20]:
```
n_iterations = 100
η = 1/2
n_lambdas = 100
lambdas = np.linspace(0, 1, n_lambdas)

result_1qbit: Benchmark_Results = benchmark_VQE(VQE_1qbit, Hamiltonian_1qbit

switch_point = 2/3
result_1qbit.switch_point = switch_point
```

```
+------------------+------------+---------------------------+
| Method           |   Time (s) |   Times Slower than Numpy |
+==================+============+===========================+
| VQE_1qbit (cold) |     2.7    |                   2484.84 |
+------------------+------------+---------------------------+
| VQE_1qbit (warm) |     0.056  |                     52.02 |
+------------------+------------+---------------------------+
| Numpy            |     0.0011 |                      1    |
+------------------+------------+---------------------------+
```

In [21]:
```
fig = plot_eigvals(result_1qbit)
plt.title('Energy eigenvalues of VQE and Numpy')
plt.savefig('figs/c_vqe_vs_numpy.pdf')
plt.savefig('selected_results/c_vqe_vs_numpy.pdf')
plt.show()
```



In [22]:
```
fig = plot_relative_error(result_1qbit)
plt.title('Relative error between VQE_1qbit and Numpy')
plt.savefig('figs/c_relative_error.pdf')
plt.show()
```



Error Analysis

In [23]:
```
error_statistics(result_1qbit)
```

Metric	Error (%)
Mean	0.001%
Median	3e-14%
Max	0.04%
Min	0%
Std	0.006%

Repeating the VQE calculation using qiskit's VQE algorithm

Hamiltonian in terms of Pauli matrices:

$$H_0 = \mathcal{E} I + \Omega \sigma_z$$

with $\mathcal{E} = (E_1 + E_2)/2$ and $\Omega = (E_1 - E_2)/2$.

$$H_I = cI + \omega_z \sigma_z + \omega_x \sigma_x$$

with $c = (V11 + V22)/2$, $\omega_z = (V11 - V22)/2$ and $\omega_x = V12 = V21$.

The total Hamiltonian is then:

$$H = H_0 + \lambda H_I$$

Circuit

In [24]:

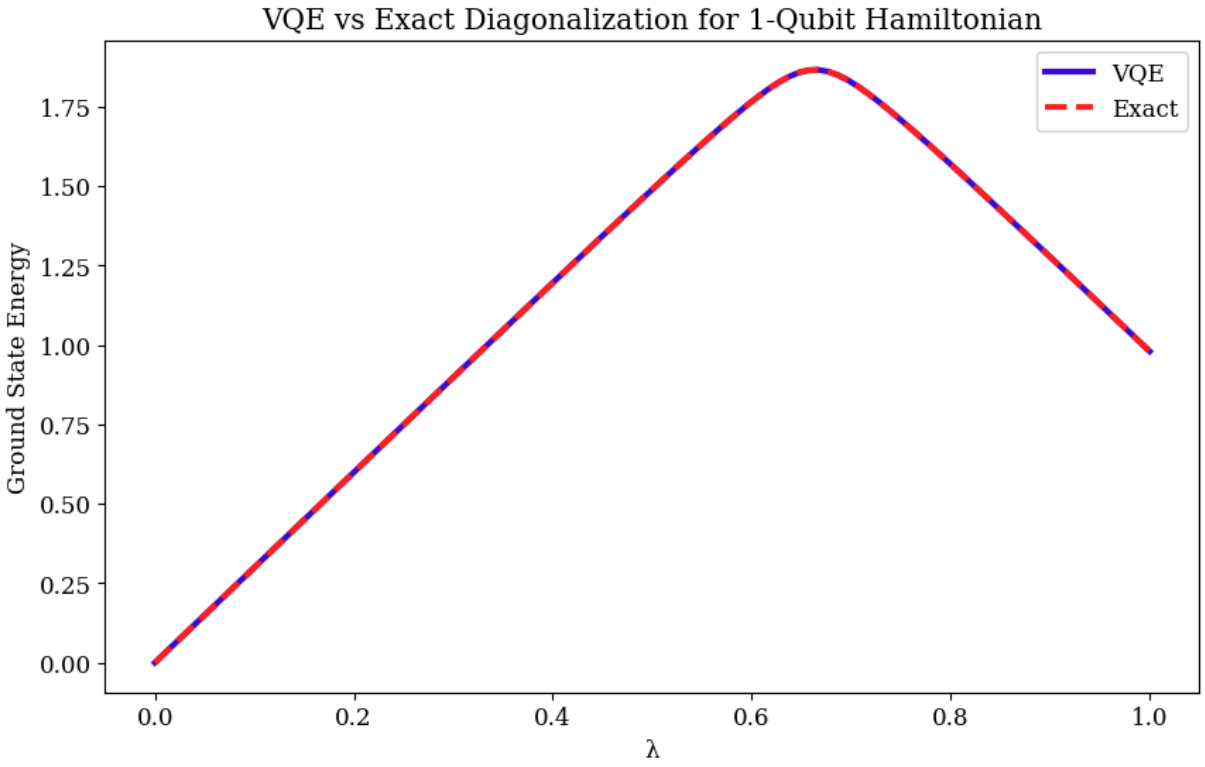
```
from tqdm import tqdm

def Hamiltonian_1qbit_circuit(λ: float) -> SparsePauliOp:
    """
    Creates a 1-qubit Hamiltonian in Qiskit's representation

    Parameters
    ----------
    λ : float
        Interaction strength

    Returns
    -------
    SparsePauliOp
        Hamiltonian as a sparse Pauli operator
    """
    # Parameters from Hamiltonian_1qbit
    E1, E2 = 0, 4
    E = (E1 + E2) / 2  # = 2
    Ω = (E1 - E2) / 2  # = -2

    V11 = 3
    V22 = -V11
    V12 = V21 = 0.2
    c   = (V11 + V22) / 2  # = 0
    ω_z = (V11 - V22) / 2  # = 3
    ω_x = V12  # = 0.2

    # Construct Hamiltonian terms
    # H = E*I + Ω*σ_z + λ*(c*I + ω_z*σ_z + ω_x*σ_x)
    # H = E*I + (Ω + λ*ω_z)*σ_z + λ*ω_x*σ_x

    hamiltonian = SparsePauliOp.from_list([
        ("I", E + λ*c),       # Identity term
        ("Z", Ω + λ*ω_z),     # Z term
        ("X", λ*ω_x)          # X term
    ])


    return hamiltonian

def create_ansatz_circuit() -> QuantumCircuit:
    """
    Creates a parameterized ansatz circuit for 1-qubit VQE

    Returns
    -------
    QuantumCircuit
        Parameterized quantum circuit
    """
    θ = Parameter('θ')
```

```
    φ = Parameter('φ')

    qc = QuantumCircuit(1)
    qc.rx(θ, 0)
    qc.ry(φ, 0)

    return qc

def run_vqe(λ: float) -> float:
    """
    Run VQE algorithm for a 1-qubit system

    Parameters
    ----------
    λ : float
        Interaction strength

    Returns
    -------
    float
        Ground state energy
    """
    # Create Hamiltonian
    hamiltonian = Hamiltonian_1qbit_circuit(λ)

    # Create ansatz circuit
    ansatz = create_ansatz_circuit()

    # Set up Gradient Descent optimizer
    optimizer = AQGD(maxiter=100)

    # Run VQE
    estimator = Estimator()
    vqe = VQE(estimator, ansatz, optimizer)
    result = vqe.compute_minimum_eigenvalue(hamiltonian)

    return result.eigenvalue.real

# Compare with exact solution
def compare_vqe_with_exact(λ_values):
    """
    Compare VQE results with exact diagonalization

    Parameters
    ----------
    λ_values : list or ndarray
        List of λ values to compute eigenvalues for

    Returns
    -------
    tuple
        (vqe_energies, exact_energies)
    """
    vqe_energies = []
    exact_energies = []
```

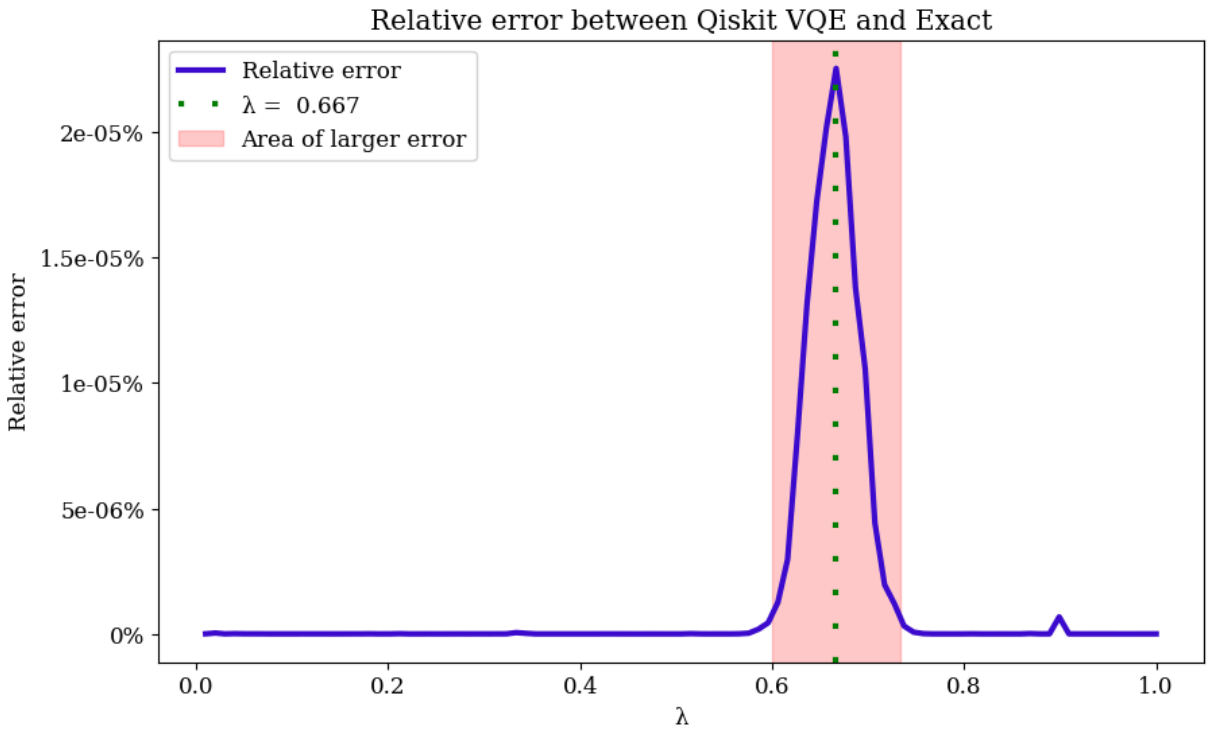
```
    for λ in tqdm(λ_values):
        # VQE solution
        vqe_energy = run_vqe(λ)
        vqe_energies.append(vqe_energy)

        # Exact solution using NumPyMinimumEigensolver
        hamiltonian = Hamiltonian_1qbit_circuit(λ)
        exact_solver = NumPyMinimumEigensolver()
        result = exact_solver.compute_minimum_eigenvalue(hamiltonian)
        exact_energies.append(result.eigenvalue.real)


    return vqe_energies, exact_energies

lambdas = np.linspace(0, 1, 100)
filterwarnings("ignore", category=DeprecationWarning) # Ignore DeprecationWa
vqe_results, exact_results = compare_vqe_with_exact(lambdas)
filterwarnings("default", category=DeprecationWarning) # Turn warning back o
```

```
100%|██████████| 100/100 [00:12<00:00,  7.94it/s]
```

In [25]:
```
# Plot the results
plt.plot(lambdas, vqe_results, '-', label='VQE')
plt.plot(lambdas, exact_results, '--', label='Exact')
plt.xlabel('λ')
plt.ylabel('Ground State Energy')
plt.title('VQE vs Exact Diagonalization for 1-Qubit Hamiltonian')
plt.legend()
plt.savefig('figs/d_vqe_qiskit_vs_exact.pdf')
plt.savefig('selected_results/d_vqe_qiskit_vs_exact.pdf')
plt.show()
```



In [26]:
```
result_1qbit_qk = Benchmark_Results(np.array(vqe_results), np.array(exact_re
fig = plot_relative_error(result_1qbit_qk)
plt.title('Relative error between Qiskit VQE and Exact')
plt.savefig('figs/d_relative_error.pdf')
plt.show()
```



In [27]:
```
error_statistics(result_1qbit_qk)
```

Metric	Error (%)
Mean	1e-06%
Median	1e-09%
Max	2e-05%
Min	1e-12%
Std	4e-06%

Conclusion

- As we can see, the VQE method is able to approximate the eigenvalues of the Hamiltonian matrix, with a relative error of $\approx 0.04\%$ with our own VQE implementation, and $\approx 0.00003\%$ with qiskit's VQE implementation. Qiskit was a lot slower than our implementation, but it was also more accurate.
- Larger error around the $\lambda = 2/3$ region. This makes sense as the energy eigenstates are close in energy, making it harder to distinguish between them.

d)

Functions

In [28]:

```
@njit
def Hamiltonian_2qbit(λ: float) -> Array4x4_c:
    '''
    Creates the Hamiltonian for a given interaction strength λ.

    Parameters
    ----------
        λ: float
            The interaction strength

    Returns
    -------
        H: Array4x4_c
            The complex 4x4 Hamiltonian matrix
    '''
    ε00, ε10, ε01, ε11 = 0.0, 2.5, 6.5, 7.0
    # np.diag not supported by numba
    H0: Array2x2 = np.array([[ε00, 0, 0, 0],
                             [0, ε10, 0, 0],
                             [0, 0, ε01, 0],
                             [0, 0, 0, ε11]], dtype=complex128)
    Hx = 2
    Hz = 3
    σ_x, σ_y, σ_z = pauli()
    HI: Array2x2 = tensor_prod(Hx*σ_x, σ_x) + tensor_prod(Hz*σ_z, σ_z)

    H:  Array2x2 = H0 + λ*HI

    return H

def density_matrix_groundstate(λ: float) -> Array4x4:
    '''
    Creates the density matrix of the lowest energy state

    Parameters
    ----------
        λ: float
            The interaction strength

    Returns
    -------
        ρ0: Array4x4
            The density matrix of the lowest energy state
    '''
    H = Hamiltonian_2qbit(λ)
    ψ_0: Array4D = np.linalg.eigh(H)[1][:, 0]

    ρ0: Array4x4 = np.outer(ψ_0, ψ_0.conj())
```

```
    return ρ0

def partial_trace(qubit: Indexing_2qbit, ρ: Array4x4) -> float:
    '''
    Partial trace over qubit

    Parameters
    ----------
        qubit: int
            Which qubit to trace over. Uses 0-based indexing
        ρ: Array4x4
            The density matrix

    Returns
    -------
        Tr(ρ_partial): float
            The partial trace of the density matrix
    '''
    q0, q1 = create_system_vectors(1)
    I_2 = np.eye(2)

    if qubit == 0:
        op0 = tensor_prod(q0, I_2)
        op1 = tensor_prod(q1, I_2)

    elif qubit == 1:
        op0 = tensor_prod(I_2, q0)
        op1 = tensor_prod(I_2, q1)

    else:
        raise ValueError('qubit must be 0 or 1')

    return op0.conj() @ ρ @ op0.T + op1.conj() @ ρ @ op1.T


def entropy(λ: float, ε: float = 1e-12) -> float:
    '''
    Calculates the entropy of the reduced density matrix

    Parameters
    ----------
        λ: float
            The interaction strength
        ε: float (optional)
            Small value to avoid log(0). Default is 1e-12

    Returns
    -------
        S: float
            The entropy of the reduced density matrix
    '''
    ρ0 = density_matrix_groundstate(λ)
    ρ_A = partial_trace(0, ρ0)
    S = -np.trace(ρ_A @ np.log2(ρ_A + ε))

    # Sanity check
```

```
    assert np.iscomplex(S) == False, f'Entropy is complex. Something went wr
    return S.real
```

Analytical Solution

Using SymPy

In [29]:
```
ε00, ε01, ε10, ε11 = sp.symbols('ε00 ε01 ε10 ε11')
λ = sp.symbols('λ')
Hx, Hz = sp.symbols('H_x H_z')
H = sp.Matrix([[ε00 + λ*Hz, 0         , 0         , λ*Hx],
               [0         , ε10 - λ*Hz, λ*Hx      , 0],
               [0         , λ*Hx      , ε01 - λ*Hz, 0],
               [λ*Hx      , 0         , 0         , ε11 + λ*Hz]])

# Sometimes finding the eigenvectors and values hangs.
# This usually takes 5 seconds (on my machine)
# If it takes longer, interrupt the cell and run it again
eigvecs_and_vals = H.eigenvects(simplify=True)

eigvals = [eigvec[0] for eigvec in eigvecs_and_vals]
eigvecs = [eigvec[2][0] for eigvec in eigvecs_and_vals]
```

In [30]:
```
Hx = 2
Hz = 3
ε00, ε10, ε01, ε11 = 0, 2.5, 6.5, 7

# Evaluate eigenvalues at λ = 0
eigvals_at_lambda_0 = [eigval.subs({'Hx': Hx, 'Hz': Hz, 'ε00': ε00, 'ε10': ε

# Sort eigenvectors by their respective eigenvalues at λ = 0
eigvecs = [eigvec for _, eigvec in sorted(zip(eigvals_at_lambda_0, eigvecs),


for i, (eigval, eigvec) in enumerate(zip(eigvals, eigvecs)):
    print(f'Eigenvalue {i}:')
    display(sp.simplify(eigval))
    print(f'Eigenvector {i}:')
    display(sp.simplify(eigvec))
    print('--'*24)
    print()
```

```
Eigenvalue 0:
```

$$-H_z\lambda + \frac{\varepsilon_{01}}{2} + \frac{\varepsilon_{10}}{2} - \frac{\sqrt{4H_x^2\lambda^2 + \varepsilon_{01}^2 - 2\varepsilon_{01}\varepsilon_{10} + \varepsilon_{10}^2}}{2}$$

```
Eigenvector 0:
```

$$\begin{bmatrix} \frac{\varepsilon_{00}-\varepsilon_{11}-\sqrt{4H_x^2\lambda^2+\varepsilon_{00}^2-2\varepsilon_{00}\varepsilon_{11}+\varepsilon_{11}^2}}{2H_x\lambda} \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Eigenvalue 1:

$$-H_z\lambda+\frac{\varepsilon_{01}}{2}+\frac{\varepsilon_{10}}{2}+\frac{\sqrt{4H_x^2\lambda^2+\varepsilon_{01}^2-2\varepsilon_{01}\varepsilon_{10}+\varepsilon_{10}^2}}{2}$$

Eigenvector 1:

$$\begin{bmatrix} 0 \\ \frac{-\varepsilon_{01}+\varepsilon_{10}-\sqrt{4H_x^2\lambda^2+\varepsilon_{01}^2-2\varepsilon_{01}\varepsilon_{10}+\varepsilon_{10}^2}}{2H_x\lambda} \\ 1 \\ 0 \end{bmatrix}$$

Eigenvalue 2:

$$H_z\lambda+\frac{\varepsilon_{00}}{2}+\frac{\varepsilon_{11}}{2}-\frac{\sqrt{4H_x^2\lambda^2+\varepsilon_{00}^2-2\varepsilon_{00}\varepsilon_{11}+\varepsilon_{11}^2}}{2}$$

Eigenvector 2:

$$\begin{bmatrix} 0 \\ \frac{-\varepsilon_{01}+\varepsilon_{10}+\sqrt{4H_x^2\lambda^2+\varepsilon_{01}^2-2\varepsilon_{01}\varepsilon_{10}+\varepsilon_{10}^2}}{2H_x\lambda} \\ 1 \\ 0 \end{bmatrix}$$

Eigenvalue 3:

$$H_z\lambda+\frac{\varepsilon_{00}}{2}+\frac{\varepsilon_{11}}{2}+\frac{\sqrt{4H_x^2\lambda^2+\varepsilon_{00}^2-2\varepsilon_{00}\varepsilon_{11}+\varepsilon_{11}^2}}{2}$$

Eigenvector 3:

$$\begin{bmatrix} \frac{\varepsilon_{00}-\varepsilon_{11}+\sqrt{4H_x^2\lambda^2+\varepsilon_{00}^2-2\varepsilon_{00}\varepsilon_{11}+\varepsilon_{11}^2}}{2H_x\lambda} \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Using the Results from Above

In [31]:

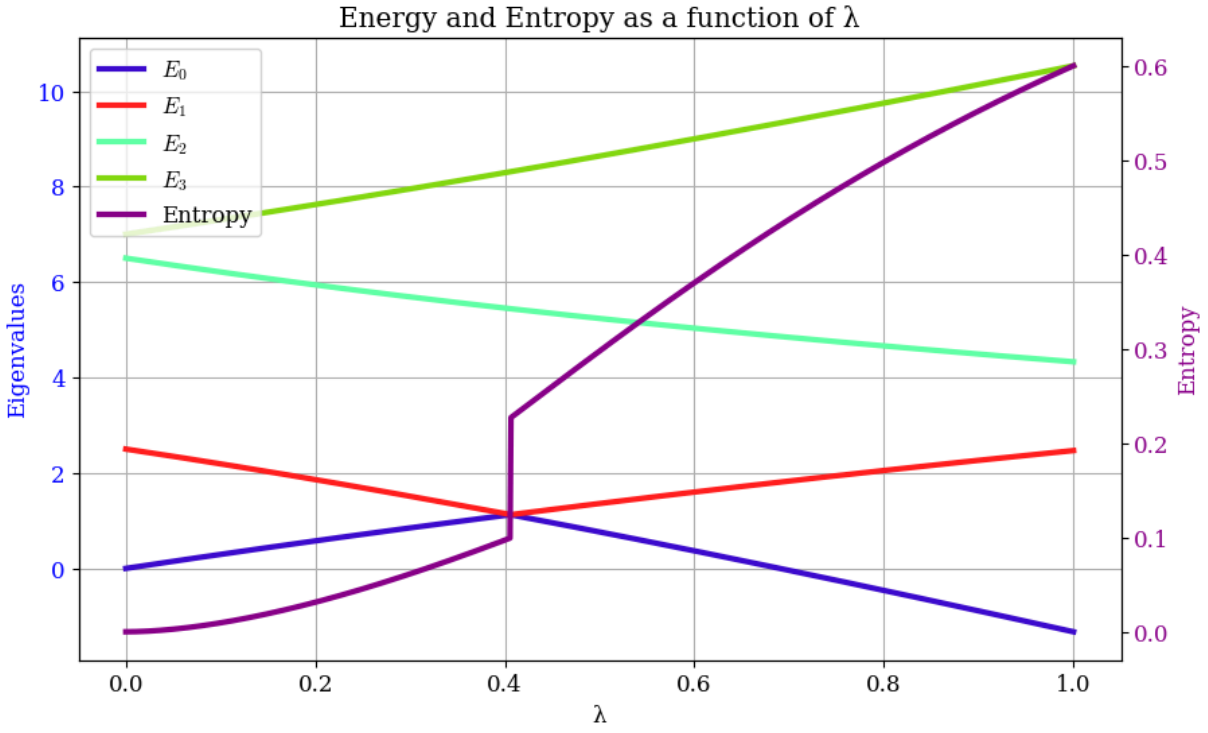
```
def analytical_energy_eigenstates(λ: float) -> tuple[Array4D, Array4D, Array
    '''
    Calculates the energy eigenstates of the Hamiltonian using the analytica

    Parameters
    ----------
        λ: float
            The interaction strength

    Returns
    -------
        eigenstates: tuple[Array4x4, Array4x4, Array4x4, Array4x4]
            The energy eigenstates. The order is the same as the energy eige
    '''
    Hx = 2
    Hz = 3
    ε00, ε10, ε01, ε11 = 0, 2.5, 6.5, 7
    q00, q01, q10, q11 = create_system_vectors(2)

    sqrt1 = np.sqrt(4*(Hx*λ)**2 + ε01**2 - 2*ε01*ε10 + ε10**2)
    sqrt2 = np.sqrt(4*(Hx*λ)**2 + ε00**2 - 2*ε00*ε11 + ε11**2)


    filterwarnings('ignore', category=RuntimeWarning) # Suppress RuntimeWarr

    v0: Array4D_c = q00 * (ε00 - ε11 - sqrt2)/(2*Hx*λ) + \
                    q01 * 0 +                           \
                    q10 * 0 +                           \
                    q11 * 1

    v1: Array4D_c = q00 * 0 +                           \
                    q01 * (ε10 - ε01 - sqrt1)/(2*Hx*λ) + \
                    q10 * 1 +                           \
                    q11 * 0

    v2: Array4D_c = q00 * 0 +                           \
                    q01 * (ε10 - ε01 + sqrt1)/(2*Hx*λ) + \
                    q10 * 1 +                           \
                    q11 * 0


    v3: Array4D_c = q00 * (ε00 - ε11 + sqrt2)/(2*Hx*λ) + \
                    q01 * 0 +                           \
                    q10 * 0 +                           \
                    q11 * 1

    filterwarnings('default', category=RuntimeWarning) # Reset warnings

    # Normalizing the vectors
    v0: Array4D = v0 / np.linalg.norm(v0)
    v1: Array4D = v1 / np.linalg.norm(v1)
    v2: Array4D = v2 / np.linalg.norm(v2)
    v3: Array4D = v3 / np.linalg.norm(v3)
```

```
    return v0, v1, v2, v3


def analytical_energy_eigenvalues(λ: float) -> tuple[float, float, float, fl
    '''
    Calculates the energy eigenvalues of the Hamiltonian using the analytica

    Parameters
    ----------
        λ: float
            The interaction strength

    Returns
    -------
        eigenvalues: tuple[float, float, float, float]
            The energy eigenvalues. The order is the same as the energy eige
    '''
    Hx = 2
    Hz = 3
    ε00, ε10, ε01, ε11 = 0, 2.5, 6.5, 7
    sqrt1 = np.sqrt(4*(Hx*λ)**2  + ε01**2 - 2*ε01*ε10 + ε10**2)
    sqrt2 = np.sqrt(4*Hx*Hz*λ**2 + ε00**2 - 2*ε00*ε11 + ε11**2)

    eigval_0 = 1/2 * (ε00 + ε11 - sqrt2 + 2*Hz*λ)
    eigval_1 = 1/2 * (ε01 + ε10 - sqrt1 - 2*Hz*λ)
    eigval_2 = 1/2 * (ε01 + ε10 + sqrt1 - 2*Hz*λ)
    eigval_3 = 1/2 * (ε00 + ε11 + sqrt2 + 2*Hz*λ)

    return eigval_0, eigval_1, eigval_2, eigval_3


def entropy_state(state: Literal[0, 1, 2, 3], λ: float, ε: float = 1e-12) ->
    '''
    Calculates the entropy for a given energy eigenstate

    Parameters
    ----------
        state: int
            The state to find the entropy of. Uses 0-based indexing
        λ: float
            The interaction strengths
        ε: float (optional)
            Small value to avoid log(0). Default is 1e-12
    Returns
    -------
        S: float
            The entropy of the reduced density matrix for the original grour
    '''

    ψ: Array4D  = analytical_energy_eigenstates(λ)[state]
    ρ: Array4x4 = np.outer(ψ, ψ.conj())

    ρ_A = partial_trace(0, ρ) # Does not matter which qubit we trace over
    S = -np.trace(ρ_A @ np.log2(ρ_A + ε))
```

```
    # Sanity check
    assert np.iscomplex(S) == False, f'Entropy is complex. Something went wr
    return S.real
```

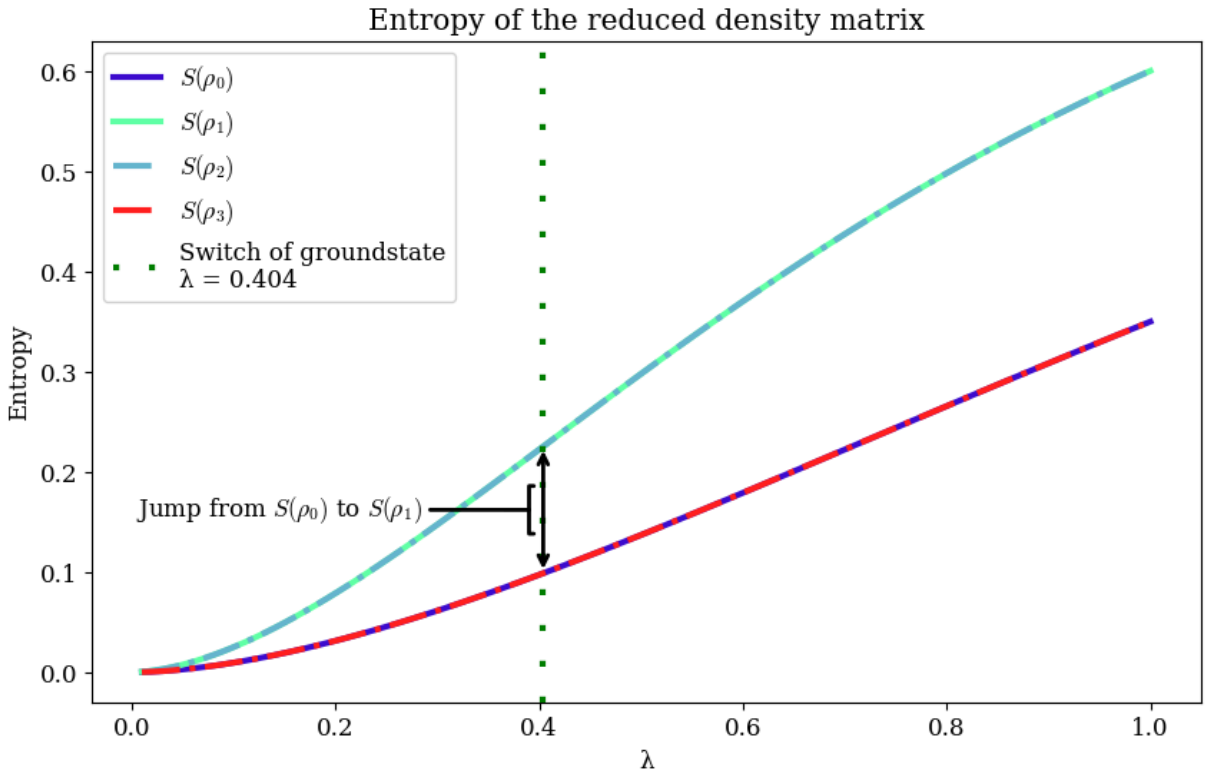
Plotting Energy and Entropy

In [32]:
```
n_lambdas = 1000
lambdas = np.linspace(0, 1, n_lambdas)
energy_eigvals = [np.linalg.eigvalsh(Hamiltonian_2qbit(λ)) for λ in lambdas]
entropies = [entropy(λ) for λ in lambdas]

plt.plot(lambdas, energy_eigvals, label=['$E_0$', '$E_1$', '$E_2$', '$E_3$']
lines_energy, labels_energy = plt.gca().get_legend_handles_labels()
plt.xlabel('λ')
plt.ylabel('Eigenvalues', color='blue')
plt.yticks(color='blue')
plt.grid()

plt.twinx()

plt.plot(lambdas, entropies, color='darkmagenta', label='Entropy')
lines_entropy, labels_entropy = plt.gca().get_legend_handles_labels()
plt.ylabel('Entropy', color='darkmagenta')
plt.yticks(color='darkmagenta')
plt.title('Energy and Entropy as a function of λ')
plt.legend(lines_energy + lines_entropy, labels_energy + labels_entropy)
plt.savefig('figs/d_energy_entropy.pdf')
plt.savefig('selected_results/d_energy_entropy.pdf')
plt.show()
```



In [33]:

```
n_lambdas = 100
lambdas = np.linspace(0, 1, n_lambdas)

entropy_0 = [entropy_state(0, λ) for λ in lambdas]
entropy_1 = [entropy_state(1, λ) for λ in lambdas]
entropy_2 = [entropy_state(2, λ) for λ in lambdas]
entropy_3 = [entropy_state(3, λ) for λ in lambdas]

energy_eigvals = np.array([np.linalg.eigvalsh(Hamiltonian_2qbit(λ)).real for

E0 = energy_eigvals[:, 0]
E1 = energy_eigvals[:, 1]

switch_point_idx = np.argmin(np.abs(E0 - E1))
gap = entropy_2[switch_point_idx] - entropy_0[switch_point_idx]

plt.plot(lambdas, entropy_0, label=r'$S(ρ_0)$', linewidth = 3, linestyle='-'
plt.plot(lambdas, entropy_1, label=r'$S(ρ_1)$', linewidth = 3, linestyle='-'
plt.plot(lambdas, entropy_2, label=r'$S(ρ_2)$', linewidth = 3, linestyle='-.
plt.plot(lambdas, entropy_3, label=r'$S(ρ_3)$', linewidth = 3, linestyle='-.
plt.axvline(x=lambdas[switch_point_idx], color='green', linestyle=(0, (1, 5)
plt.ylabel('Entropy')
plt.xlabel('λ')
plt.title('Entropy of the reduced density matrix')

plt.annotate(text="",
             xy=(lambdas[switch_point_idx], entropy_0[switch_point_idx]),
             xytext=(lambdas[switch_point_idx], entropy_0[switch_point_idx]
             arrowprops=dict(arrowstyle='<->', lw=2)
            )

plt.annotate(text="Jump from $S(ρ_0)$ to $S(ρ_1)$",
             xy=(lambdas[switch_point_idx]-.01, entropy_0[switch_point_idx]
             xytext=(lambdas[switch_point_idx] - 0.4, entropy_0[switch_point
             arrowprops=dict(arrowstyle='-[', lw=2)
            )

plt.legend()
plt.savefig('figs/d_entropy.pdf')
plt.show()
```



Conclusion

- As the interaction strength λ increases, we see a switch in which the lowest energy state switches from $|\psi_0\rangle$ with corresponding eigenvalue E_0, to $|\psi_1\rangle$ with corresponding eigenvalue E_1.
- When calculating the entropy, we always look at the lowest energy state. After the switch from $|\psi_0\rangle$ to $|\psi_1\rangle$, we switch what state we calculate the entropy from. As these two states have different entropies, the entropy makes a sudden jump at the point of the switch.

e)

Functions

In [34]:
```
@njit
def Energy_2qbit(θ1: float, θ2: float, θ3: float, θ4: float, λ: float) -> fl
    '''
    Calculates the energy eigenvalues of the Hamiltonian for a 2-qubit syste

    Parameters
    ----------
        θ1: float
            The angle (radians) to rotate by around the x-axis of qubit 0
        θ2: float
```

```
            The angle (radians) to rotate by around the y-axis of qubit 0
        θ3: float
            The angle (radians) to rotate by around the x-axis of qubit 1
        θ4: float
            The angle (radians) to rotate by around the y-axis of qubit 1
        λ: float
            The interaction strength

    Returns
    -------
        E: float
            The energy eigenvalue (real part)
    '''
    R1:   Array2x2_c = Rx(θ1) @ Ry(θ2)
    R2:   Array2x2_c = Rx(θ3) @ Ry(θ4)
    CNOT: Array4x4_c = cnot()

    basis = np.array([1, 0, 0, 0], dtype=complex128) # |00⟩: Will be rotated
    rotated_basis: Array4x4_c = CNOT @ tensor_prod(R1, R2) @ basis
    E = rotated_basis.conj().T @ Hamiltonian_2qbit(λ) @ rotated_basis

    assert abs(E.imag) < 1e-14  , f'Energy is complex. Something went wrong:
    return E.real

@njit
def VQE_2qbit(N: int, η: float, λ: float = 0, seed: int = 2024) -> float:
    '''
    Variational Quantum Eigensolver using Gradient Descent to find the minim

    Parameters
    ----------
        N: int
            Number of iterations
        η: float
            Learning rate
        λ: float
            Interaction strength of the Hamiltonian
        seed: int
            Seed for the random number generator

    Returns
    -------
        Energy(θ1, θ2, θ3, θ4, λ): float
            The energy eigenvalue (real part)
    '''
    π = np.pi
    np.random.seed(seed)
    θ1 = 2*π*np.random.rand()
    θ2 = 2*π*np.random.rand()
    θ3 = 2*π*np.random.rand()
    θ4 = 2*π*np.random.rand()

    # More compact to rename function
    E: Callable = Energy_2qbit
    for _ in range(N):
        ΔE_Δθ1 = (E(θ1+π/2, θ2, θ3, θ4, λ) - E(θ1-π/2, θ2, θ3, θ4, λ)) / 2
```

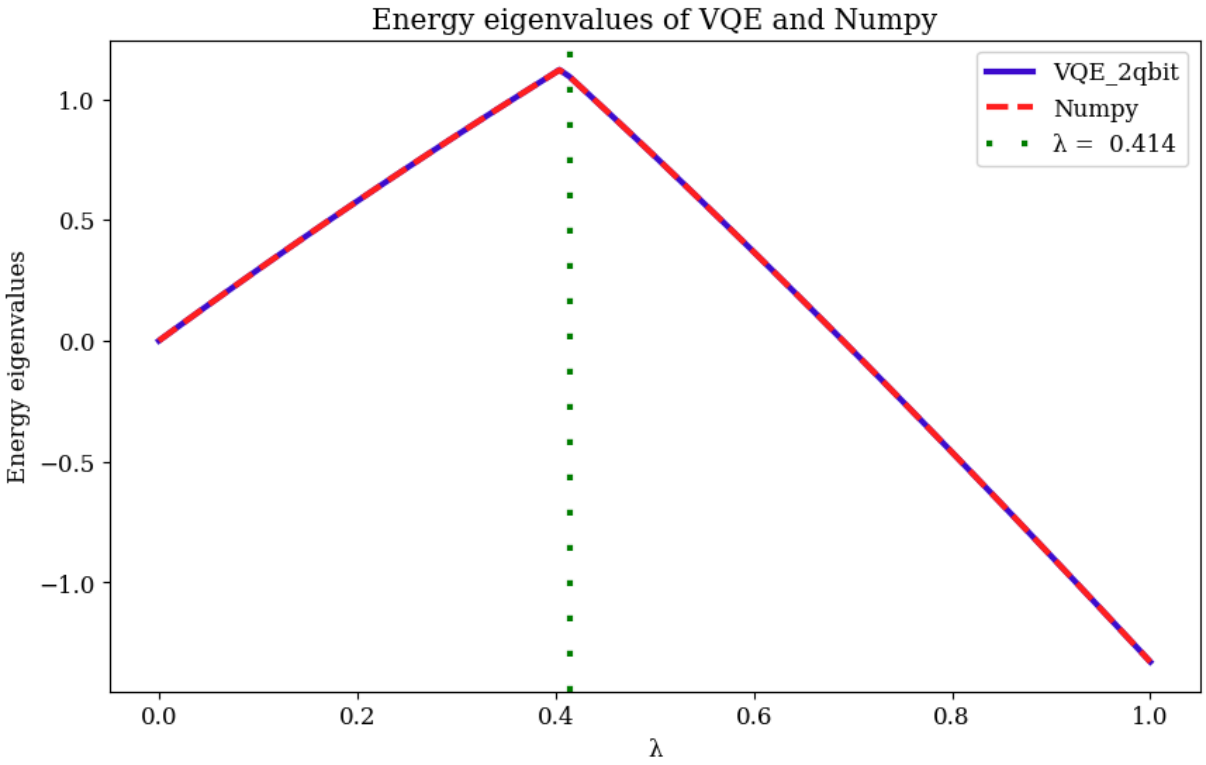
```
        ΔE_Δθ2 = (E(θ1, θ2+π/2, θ3, θ4, λ) - E(θ1, θ2-π/2, θ3, θ4, λ)) / 2
        ΔE_Δθ3 = (E(θ1, θ2, θ3+π/2, θ4, λ) - E(θ1, θ2, θ3-π/2, θ4, λ)) / 2
        ΔE_Δθ4 = (E(θ1, θ2, θ3, θ4+π/2, λ) - E(θ1, θ2, θ3, θ4-π/2, λ)) / 2

        θ1 -= η * ΔE_Δθ1
        θ2 -= η * ΔE_Δθ2
        θ3 -= η * ΔE_Δθ3
        θ4 -= η * ΔE_Δθ4

    # Using the actual function name
    E = Energy_2qbit(θ1, θ2, θ3, θ4, λ)
    return E
```

Comparing VQE and Exact Eigenvalues

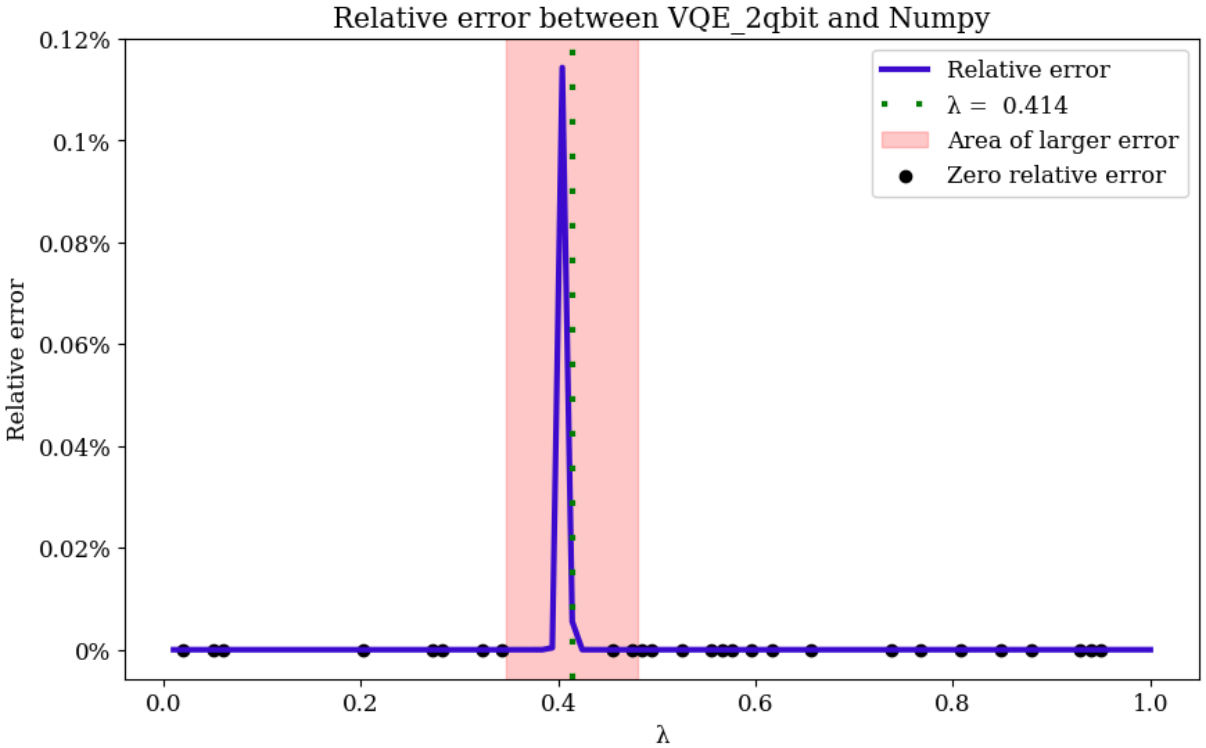
In [35]:
```
n_iterations = 400
η = 1/4
n_lambdas = 100
lambdas = np.linspace(0, 1, n_lambdas)

result_2qbit: Benchmark_Results = benchmark_VQE(VQE_2qbit, Hamiltonian_2qbit

energy_eigvals = np.array([analytical_energy_eigenvalues(λ) for λ in lambdas
E0 = energy_eigvals[:, 0]
E1 = energy_eigvals[:, 1]

switch_point_idx = np.argmin(np.abs(E0 - E1))
switch_point = lambdas[switch_point_idx]

result_2qbit.switch_point = switch_point
```

```
+------------------+------------+----------------------------+
| Method           |   Time (s) |   Times Slower than Numpy |
+==================+============+============================+
| VQE_2qbit (cold) |     2.7    |                    1951.89 |
+------------------+------------+----------------------------+
| VQE_2qbit (warm) |     1.4    |                    1037.72 |
+------------------+------------+----------------------------+
| Numpy            |     0.0014 |                          1 |
+------------------+------------+----------------------------+
```

In [36]:
```
fig = plot_eigvals(result_2qbit)
plt.title('Energy eigenvalues of VQE and Numpy')
plt.savefig('figs/e_vqe_vs_numpy.pdf')
plt.savefig('selected_results/e_vqe_vs_numpy.pdf')
plt.show()
```



In [37]:
```
fig = plot_relative_error(result_2qbit)
plt.title('Relative error between VQE_2qbit and Numpy')
plt.savefig('figs/e_relative_error.pdf')
plt.show()
```



Error Analysis

In [38]:
```
error_statistics(result_2qbit)
```

```
+----------+-------------+
| Metric   | Error (%)   |
+==========+=============+
| Mean     | 0.001%      |
| Median   | 2e-14%      |
| Max      | 0.1%        |
| Min      | 0%          |
| Std      | 0.01%       |
+----------+-------------+
```

In [39]:
```
def hamiltonian_2qbit_qiskit(λ: float) -> SparsePauliOp:
    """
    Express the 2-qubit Hamiltonian as a sum of Pauli operators for Qiskit

    Parameters
    ----------
    λ : float
        Interaction strength

    Returns
    -------
    SparsePauliOp
        Hamiltonian as Pauli operators
    """
    # Parameters from Hamiltonian_2qbit
    ε00, ε10, ε01, ε11 = 0.0, 2.5, 6.5, 7.0
    Hx = 2
    Hz = 3

    # Express H0 (diagonal matrix) in terms of Pauli operators
    # For a 2-qubit system, we use II, IZ, ZI, ZZ to represent diagonal matr

    # Calculate coefficients
    c_II = (ε00 + ε10 + ε01 + ε11) / 4  # Coefficient of II
    c_IZ = (ε00 + ε10 - ε01 - ε11) / 4  # Coefficient of IZ
    c_ZI = (ε00 - ε10 + ε01 - ε11) / 4  # Coefficient of ZI
    c_ZZ = (ε00 - ε10 - ε01 + ε11) / 4  # Coefficient of ZZ

    # Interaction term: λ * (Hx * XX + Hz * ZZ)
    c_XX = λ * Hx  # Coefficient of XX
    c_ZZ_interaction = λ * Hz  # Additional ZZ term from interaction

    # Combine ZZ terms
    c_ZZ_total = c_ZZ + c_ZZ_interaction

    # Create the Hamiltonian as a SparsePauliOp
    hamiltonian = SparsePauliOp.from_list([
        ('II', c_II),
        ('IZ', c_IZ),
        ('ZI', c_ZI),
        ('ZZ', c_ZZ_total),
        ('XX', c_XX)
    ])
```

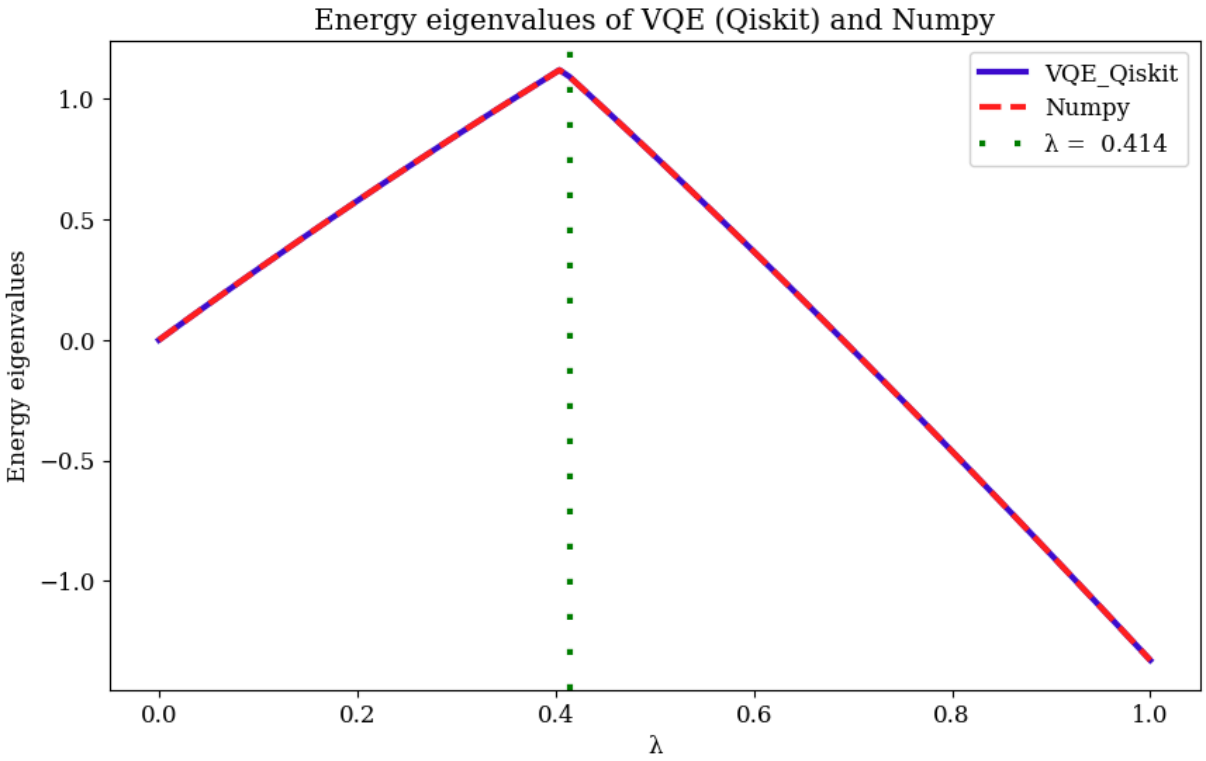
```
    return hamiltonian

def create_2qubit_ansatz() -> QuantumCircuit:
    """
    Create a parameterized ansatz for 2-qubit VQE
    Replicating the structure used in Energy_2qbit

    Returns
    -------
    QuantumCircuit
        Parameterized quantum circuit
    """
    # Define parameters
    θ1 = Parameter('θ1')
    θ2 = Parameter('θ2')
    θ3 = Parameter('θ3')
    θ4 = Parameter('θ4')

    # Create circuit
    qc = QuantumCircuit(2)

    # Apply Rx and Ry gates to each qubit
    qc.rx(θ1, 0)
    qc.ry(θ2, 0)
    qc.rx(θ3, 1)
    qc.ry(θ4, 1)

    # Apply CNOT gate
    qc.cx(0, 1)

    return qc

def run_2qubit_vqe(λ: float, max_iterations: int = 10_00) -> float:
    """
    Run VQE for the 2-qubit system with given interaction strength λ

    Parameters
    ----------
    λ : float
        Interaction strength
    max_iterations : int, optional
        Maximum number of optimizer iterations, by default 100

    Returns
    -------
    float
        Ground state energy
    """
    # Create Hamiltonian
    hamiltonian = hamiltonian_2qbit_qiskit(λ)

    # Create ansatz
    ansatz = create_2qubit_ansatz()

    # Set up optimizer
    optimizer = COBYLA(maxiter=max_iterations)
```

```
    # Create estimator
    estimator = Estimator()

    # Run VQE
    vqe = VQE(estimator, ansatz, optimizer)
    result = vqe.compute_minimum_eigenvalue(hamiltonian)

    return result.eigenvalue.real

def compare_vqe_exact(λ_values):
    """
    Compare VQE results with exact diagonalization for range of λ values

    Parameters
    ----------
    λ_values : list or array
        List of λ values to evaluate

    Returns
    -------
    tuple
        (vqe_energies, exact_energies)
    """
    vqe_energies = []
    exact_energies = []

    for λ in tqdm(λ_values):
        # Run VQE
        vqe_energy = run_2qubit_vqe(λ)
        vqe_energies.append(vqe_energy)

        # Run exact diagonalization
        hamiltonian = hamiltonian_2qbit_qiskit(λ)
        exact_solver = NumPyMinimumEigensolver()
        result = exact_solver.compute_minimum_eigenvalue(hamiltonian)
        exact_energies.append(result.eigenvalue.real)

    return vqe_energies, exact_energies

# Example usage:
λ_values = np.linspace(0, 1, 100)
filterwarnings("ignore", category=DeprecationWarning) # Ignore DeprecationWa
vqe_results, exact_results = compare_vqe_exact(λ_values)
filterwarnings("default", category=DeprecationWarning) # Turn warning back o

result_2qbit_qk = Benchmark_Results(np.array(vqe_results), np.array(exact_re
```

```
100%|██████████| 100/100 [00:20<00:00,  4.88it/s]
```

In [40]:

```
fig = plot_eigvals(result_2qbit_qk)
plt.title('Energy eigenvalues of VQE (Qiskit) and Numpy')
plt.savefig('figs/e_vqe_qiskit_vs_exact.pdf')
plt.savefig('selected_results/e_vqe_qiskit_vs_exact.pdf')
plt.show()
```



In [41]:
```
error_statistics(result_2qbit_qk)
```

```
+----------+-------------+
| Metric   | Error (%)   |
+==========+=============+
| Mean     | 1e+71%      |
| Median   | 3e-06%      |
| Max      | 1e+73%      |
| Min      | 3e-07%      |
| Std      | 1e+72%      |
+----------+-------------+
```

Conclusion

- The VQE method was 1000-2000 times slower than using numpy, as opposed to 50-80 times slower in the 1 qubit case.
  - This might not be surprising as one needs to preform the gradient descent which can't be done in parallel
  - The 2 qubit case involves twice as large matrices and vectors.
- There was about one order of magnitude difference in the performance of the VQE method between the 1 and 2 qubit case, compared to using numpy.
- The algorithm could be improved by doing more iterations if the interaction strength λ is near the point where the eigenvalues switch. This is done in the qiskit implementation.

f)

Defining the Hamiltonian for $J = 1$

We first look at how the quasispin operators act on a state on a state $\ket{j, m_j}$:

$$
\begin{aligned}
J_+\ket{j, m_j} &= \sqrt{j(j+1) - m_j(m_j+1)}\ket{j, m_j+1} \\
J_-\ket{j, m_j} &= \sqrt{j(j+1) - m_j(m_j-1)}\ket{j, m_j-1} \\
J_z\ket{j, m_j} &= m_j\ket{j, m_j}
\end{aligned}
$$

We then write then write out the possible combinations of m_j values for $J = 1$ as a matrix:

$$
J_z = \begin{pmatrix}
\bra{1, -1}J_z\ket{1, -1} & \bra{1, -1}J_z\ket{1, 0} & \bra{1, -1}J_z\ket{1, 1} \\
\bra{1, 0}J_z\ket{1, -1} & \bra{1, 0}J_z\ket{1, 0} & \bra{1, 0}J_z\ket{1, 1} \\
\bra{1, 1}J_z\ket{1, -1} & \bra{1, 1}J_z\ket{1, 0} & \bra{1, 1}J_z\ket{1, 1}
\end{pmatrix}
$$

With an orthonormal basis, we are guaranteed that the matrix is diagonal. Knowing $J_z\ket{1, 0} = 0$, we get the final expression:

$$
J_z = \begin{pmatrix}
-\hbar & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & \hbar
\end{pmatrix}
$$

We do the same for the J_+^2:

$$
J_+^2 = \begin{pmatrix}
\bra{1, -1}J_+^2\ket{1, -1} & \bra{1, -1}J_+^2\ket{1, 0} & \bra{1, -1}J_+^2\ket{1, 1} \\
\bra{1, 0}J_+^2\ket{1, -1} & \bra{1, 0}J_+^2\ket{1, 0} & \bra{1, 0}J_+^2\ket{1, 1} \\
\bra{1, 1}J_+^2\ket{1, -1} & \bra{1, 1}J_+^2\ket{1, 0} & \bra{1, 1}J_+^2\ket{1, 1}
\end{pmatrix}
$$

Which results in:

$$
J_+^2 = \begin{pmatrix}
0 & 0 & 2\hbar \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
$$

And at last for J_-^2:

$$
J_-^2 = \begin{pmatrix}
\bra{1, -1}J_-^2\ket{1, -1} & \bra{1, -1}J_-^2\ket{1, 0} & \bra{1, -1}J_-^2\ket{1, 1} \\
\bra{1, 0}J_-^2\ket{1, -1} & \bra{1, 0}J_-^2\ket{1, 0} & \bra{1, 0}J_-^2\ket{1, 1} \\
\bra{1, 1}J_-^2\ket{1, -1} & \bra{1, 1}J_-^2\ket{1, 0} & \bra{1, 1}J_-^2\ket{1, 1}
\end{pmatrix}
$$

Which results in:

$$J_-^2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 2\hbar & 0 & 0 \end{pmatrix}$$

We define $\hbar = 1$ and using $H_0 = \epsilon J_z$ and $H_1 = -V\left(J_+^2 + J_-^2\right)/2$, we get the Hamiltonian matrix for $J = 1$:

$$H = \begin{pmatrix} -\epsilon & 0 & -V \\ 0 & 0 & 0 \\ -V & 0 & \epsilon \end{pmatrix}$$

Rewriting the $J = 1$ Hamiltonian with Pauli Matrices

In [42]:
```
filterwarnings("ignore", category=ComplexWarning)
X, _, Z = map(np.astype, pauli(), [int, complex128, int]) # Convert to int t
filterwarnings("default", category=ComplexWarning)

I_2 = sp.Identity(2)

ZZ = tensor_prod(Z, Z)
ZI = tensor_prod(Z, I_2)
XI = tensor_prod(X, I_2)
XZ = tensor_prod(X, Z)

ϵ = sp.symbols('ϵ')
V = sp.symbols('V')
H = ϵ/2 * (ZI + ZZ) + V/2 * (XI + XZ)
H = sp.simplify(H)

print('Hamiltonian:')
display(H)
```

```
Hamiltonian:
```

$$\begin{bmatrix} \epsilon & 0 & V & 0 \\ 0 & 0 & 0 & 0 \\ V & 0 & -\epsilon & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Rewriting the $J = 2$ Hamiltonian with Pauli Matrices

We use block diagonalization to write our Hamiltonian using Pauli matrices:

$$H = \begin{pmatrix} H_1 & & \\ & & \\ & & H_2 \end{pmatrix}$$

Where H_1 have dimensions 4×4 and H_2 have dimensions 2×2. The code below implements and verifies the Hamiltonian being as expected. They will not look identical, but the lowest eigenvalues is the same, which is what we need

In [43]:
```
def Block4x4(ϵ: float, V: float) -> Array4x4_c:
    '''
    Creates the first block of the Hamiltonian

    Parameters
    ----------
        ϵ: float
            The coupling strength
        V: float
            The interaction strength

    Returns
    -------
        H: Array4x4_c
            The complex 4x4 block of the Hamiltonian
    '''
    X, Y, Z = pauli()
    I_2 = np.eye(2)

    IX = tensor_prod(I_2, X)
    XX = tensor_prod(X, X)

    YY = tensor_prod(Y, Y)

    ZI = tensor_prod(Z, I_2)
    ZZ = tensor_prod(Z, Z)
    ZX = tensor_prod(Z, X)

    sqrt6 = np.sqrt(6)
    H = -ϵ * (ZI + ZZ) + sqrt6*V/2 * (IX + XX + YY + ZX)
    return H

def Block2x2(ϵ: float, V: float) -> Array2x2_c:
    '''
    Creates the second block of the Hamiltonian

    Parameters
    ----------
        ϵ: float
            The coupling strength
        V: float
            The interaction strength

    Returns
    -------
        H: Array2x2_c
            The complex 2x2 block of the Hamiltonian
    '''
    X, _, Z = pauli()

    H = -ϵ*Z + 3*V*X
```

```
    return H

def Hamiltonian_Lipkin(ϵ: float, V: float) -> Array5x5_c:
    '''
    Creates the Hamiltonian for the Lipkin model

    Parameters
    ----------
        ϵ: float
            The coupling strength
        V: float
            The interaction strength

    Returns
    -------
        H: Array5x5_c
            The complex 5x5 Hamiltonian matrix
    '''
    H1 = Block4x4(ϵ, V)
    H2 = Block2x2(ϵ, V)

    H = np.zeros((5, 5), dtype=complex128)
    H[:4, :4] = H1
    H[3:, 3:] = H2

    return H
```

In [44]:

```
# Create symbolic representation of the Lipkin model Hamiltonian
ϵ = sp.symbols('ϵ', real=True)
V = sp.symbols('V', real=True)

sqrt6 = sp.sqrt(6)
H_standard = sp.Matrix([[   -2*ϵ,   0, sqrt6*V,   0,       0],
                        [      0,  -ϵ,       0, 3*V,       0],
                        [sqrt6*V,   0,       0,   0, sqrt6*V],
                        [      0, 3*V,       0,   ϵ,       0],
                        [      0,   0, sqrt6*V,   0,     2*ϵ]])

# Define Pauli matrices symbolically
σ_x = sp.Matrix([[0, 1], [1, 0]])
σ_y = sp.Matrix([[0, -sp.I], [sp.I, 0]])
σ_z = sp.Matrix([[1, 0], [0, -1]])
I_2 = sp.eye(2)

# Create symbolic blocks for the Hamiltonian
# First block (4x4)
IX = sp.kronecker_product(I_2, σ_x)
XX = sp.kronecker_product(σ_x, σ_x)
YY = sp.kronecker_product(σ_y, σ_y)
ZI = sp.kronecker_product(σ_z, I_2)
ZZ = sp.kronecker_product(σ_z, σ_z)
ZX = sp.kronecker_product(σ_z, σ_x)

H1 = -ϵ * (ZI + ZZ) + sqrt6*V/2 * (IX + XX + YY + ZX)

# Second block (2x2)
```

```
H2 = -ϵ*σ_z + 3*V*σ_x

# Create the full 5x5 Hamiltonian
H_lipkin = sp.zeros(5, 5)
H_lipkin[:4, :4] = H1
H_lipkin[3:, 3:] = H2

print("Standard Lipkin Model Hamiltonian:")
display(H_standard)
print()
print("Block Diagonalized Lipkin Model Hamiltonian:")
display(H_lipkin)
```

```
Standard Lipkin Model Hamiltonian:
```

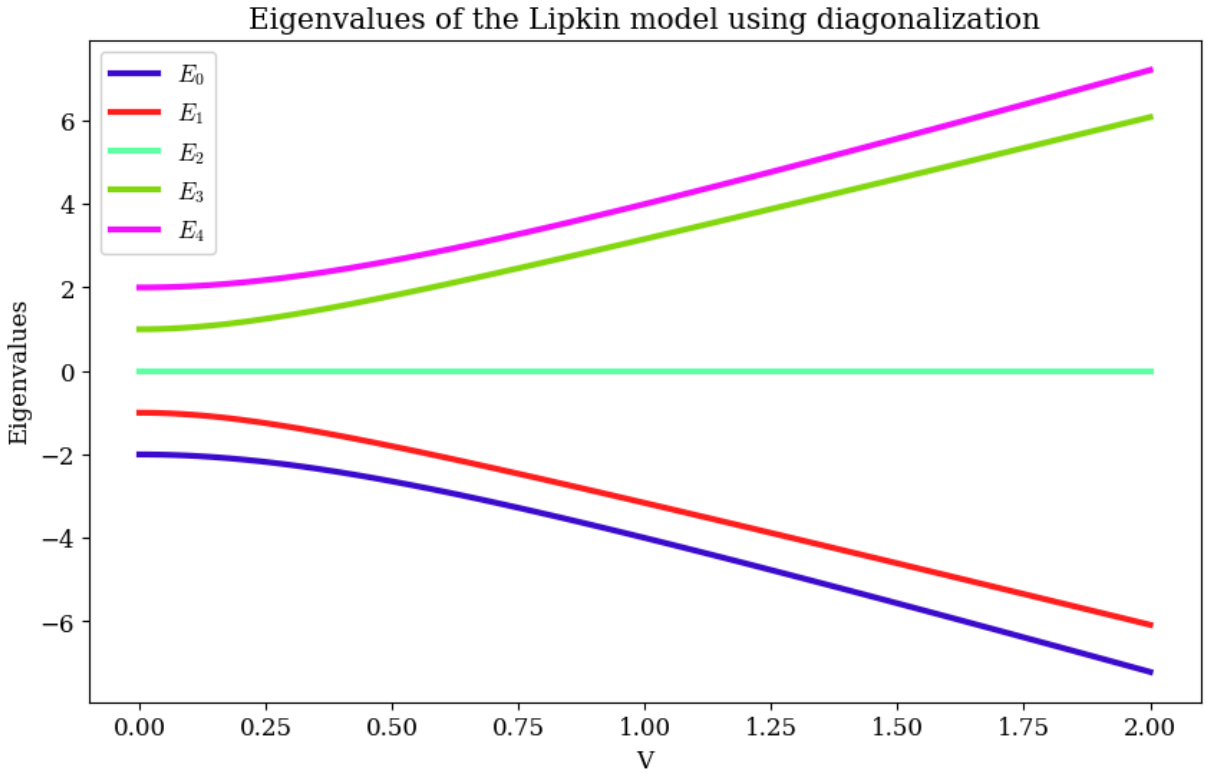
$$\begin{bmatrix} -2\epsilon & 0 & \sqrt{6}V & 0 & 0 \\ 0 & -\epsilon & 0 & 3V & 0 \\ \sqrt{6}V & 0 & 0 & 0 & \sqrt{6}V \\ 0 & 3V & 0 & \epsilon & 0 \\ 0 & 0 & \sqrt{6}V & 0 & 2\epsilon \end{bmatrix}$$

```
Block Diagonalized Lipkin Model Hamiltonian:
```

$$\begin{bmatrix} -2\epsilon & \sqrt{6}V & 0 & 0 & 0 \\ \sqrt{6}V & 0 & \sqrt{6}V & 0 & 0 \\ 0 & \sqrt{6}V & 2\epsilon & 0 & 0 \\ 0 & 0 & 0 & -\epsilon & 3V \\ 0 & 0 & 0 & 3V & \epsilon \end{bmatrix}$$

In [45]:
```
n = 100
ϵ = 1
V = np.linspace(0, 2, n)

eigevalues = []
for v in V:
    H = Hamiltonian_Lipkin(ϵ, v)
    eigevalues.append(np.linalg.eigvalsh(H))
```

In [46]:
```
plt.plot(V, eigevalues, label=['$E_0$', '$E_1$', '$E_2$', '$E_3$', '$E_4$'])
plt.xlabel('V')
plt.ylabel('Eigenvalues')
plt.title('Eigenvalues of the Lipkin model using diagonalization')
plt.legend()
plt.savefig('figs/f_lipkin_eigenvalues_classical.pdf')
plt.savefig('selected_results/f_lipkin_eigenvalues_classical.pdf')
plt.show()
```



g)

In [47]:

```python
def lipkin_hamiltonian_1qubit(ϵ: float, V: float) -> SparsePauliOp:
    """
    Creates the 1-qubit Lipkin Hamiltonian for VQE

    Parameters
    ----------
    ϵ : float
        Coupling strength
    V : float
        Interaction strength

    Returns
    -------
    SparsePauliOp
        Hamiltonian as a sparse Pauli operator
    """
    # Using the Block2x2 Hamiltonian: H = -ϵ*Z + 3*V*X
    hamiltonian = SparsePauliOp.from_list([
        ('Z', -ϵ),      # -ϵ*Z term
        ('X', 3*V)      # 3*V*X term
    ])

    return hamiltonian

def create_1qubit_ansatz() -> QuantumCircuit:
    """
    Creates a parameterized ansatz circuit for 1-qubit VQE
```

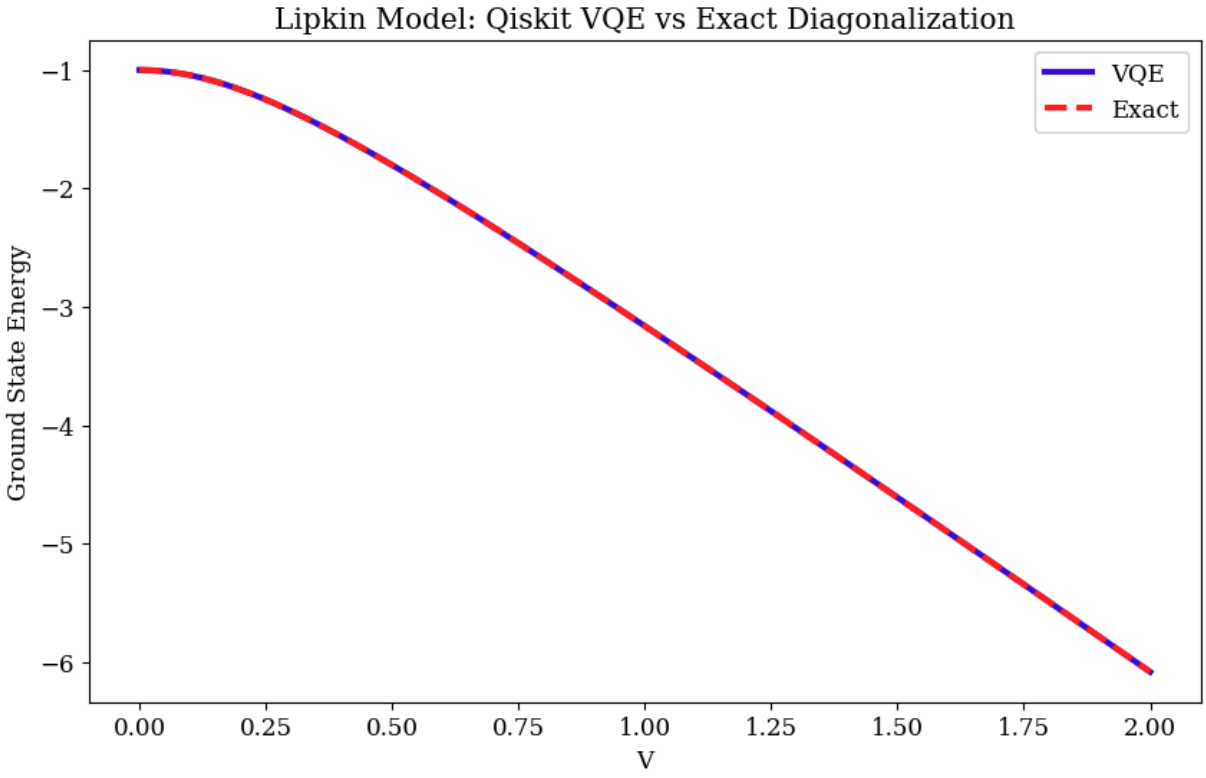
```
    Returns
    -------
    QuantumCircuit
        Parameterized quantum circuit
    """
    θ = Parameter('θ')
    φ = Parameter('φ')

    qc = QuantumCircuit(1)
    qc.rx(θ, 0)
    qc.ry(φ, 0)

    return qc

def run_lipkin_vqe(ϵ: float, V: float, max_iterations: int = 10_000) -> floa
    """
    Runs VQE for the 1-qubit Lipkin model

    Parameters
    ----------
    ϵ : float
        Coupling strength
    V : float
        Interaction strength
    max_iterations : int, optional
        Maximum optimizer iterations, by default 100

    Returns
    -------
    float
        Ground state energy
    """
    # Create Hamiltonian
    hamiltonian = lipkin_hamiltonian_1qubit(ϵ, V)

    # Create ansatz
    ansatz = create_1qubit_ansatz()

    # Set up optimizer
    optimizer = COBYLA(maxiter=max_iterations)

    # Run VQE
    estimator = Estimator()
    vqe = VQE(estimator, ansatz, optimizer)
    result = vqe.compute_minimum_eigenvalue(hamiltonian)

    return result.eigenvalue.real

# Compare with exact solution across a range of V values
def compare_lipkin_vqe_exact(ϵ: float, V_values: np.ndarray):
    """
    Compare VQE with exact diagonalization for range of V values

    Parameters
    ----------
```

```
    ϵ : float
        Coupling strength
    V_values : np.ndarray
        Array of interaction strengths to evaluate

    Returns
    -------
    tuple
        (vqe_energies, exact_energies)
    """
    vqe_energies = []
    exact_energies = []

    for V in tqdm(V_values):
        # VQE solution
        vqe_energy = run_lipkin_vqe(ϵ, V)
        vqe_energies.append(vqe_energy)

        # Exact solution using NumPyMinimumEigensolver
        hamiltonian = lipkin_hamiltonian_1qubit(ϵ, V)
        exact_solver = NumPyMinimumEigensolver()
        result = exact_solver.compute_minimum_eigenvalue(hamiltonian)
        exact_energies.append(result.eigenvalue.real)

    return vqe_energies, exact_energies

# Example usage:
ϵ = 1.0
V_values = np.linspace(0, 2, 100)
filterwarnings("ignore", category=DeprecationWarning) # Ignore DeprecationWa
vqe_results, exact_results = compare_lipkin_vqe_exact(ϵ, V_values)
filterwarnings("default", category=DeprecationWarning) #

result_lipkin = Benchmark_Results(np.array(vqe_results), np.array(exact_resu
```

```
100%|██████████| 100/100 [00:04<00:00, 23.99it/s]
```

In [48]:

```
# Plot results
plt.plot(V_values, vqe_results, label='VQE')
plt.plot(V_values, exact_results, '--', label='Exact')
plt.xlabel('V')
plt.ylabel('Ground State Energy')
plt.title('Lipkin Model: Qiskit VQE vs Exact Diagonalization')
plt.legend()
plt.savefig('figs/f_lipkin_vqe_vs_exact.pdf')
plt.savefig('selected_results/f_lipkin_vqe_vs_exact.pdf')
plt.show()
```



In [49]:
```
error_statistics(result_lipkin)
```

```
+----------+-------------+
| Metric   | Error (%)   |
+==========+=============+
| Mean     | 5e-07%      |
| Median   | 4e-07%      |
| Max      | 1e-06%      |
| Min      | 6e-08%      |
| Std      | 2e-07%      |
+----------+-------------+
```

Conclusion

- The VQE method was able to approximate the eigenvalues of the Hamiltonian matrix, with a relative error of $\approx 10^{-7}$. This was naturally slower than numpy, but a lot more performant than earlier implementation.