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```
In []: from qiskit import *
    from qiskit.circuit import Parameter,ParameterVector, Gate
    from qiskit.quantum_info import Operator
    from qiskit.circuit.library import *
    from qiskit.visualization import array_to_latex, plot_histogram
    from qutip import hilbert_dist, Qobj, fock_dm

import random

import pyswarms as ps
import pyswarms.backend as P
from pyswarms.backend.topology import Star

import numpy as np
import matplotlib.pyplot as plt
```

Introduction

To optimize a generic 3 qubit unitary, we can build it using a set of generic rotation gates composed of 11 single qubit unitaries and 4 two qubit unitaries. This process is outlined in the paper 'Optimal Implementation of Quantum Gates with Two Controls: A Detailed Proof' by Jens Palsberg and Nengkun Yu. In this assignement we used the methods in this paper to find an approximiate solution to the Toffoli gate (CCNOT) using only 4 two qubit gates. I was able to measure how close my generated Toffoli gate was to the original by comparing it to the Hilbert Schmidt distance which is outlined later.

The Toffoli Gate and the Hilbert Schmidt Distance

Here's the native Toffoli gate from qiskit:

```
In [ ]: qc = QuantumCircuit(3)
    qc.ccx(0, 1, 2)
    ccx_gate = Operator(qc).data
    array_to_latex(ccx_gate)
```

Out[]:

Hilbert Schmidt Distance

Next steps is to to have a function to measure the 'closeness' to an approximate matrix. This can be done simply with the Hilbert Schmidt Distance. This is given by the following fromula from Jens' paper 'Approximate Quantum Computing':

$$d(U,V) = \sqrt{1-rac{\|Tr(U^\dagger V)\|^2}{N^2}}$$

Where Tr(U) is the trace of U and $N=2^n$. This will give us the absolute value of the Hilbert Schmidt distance (a real value), which will be easy to optimize around. I've defined this function below in <code>my_hilbert_schmidt_distance</code>. I've also defined an additional function <code>get_hilbert_shmidt_distance</code> which returns the 2d imaginary Hilbert Schmidt distance. This definition comes from the qutip library and I use it later to do some further optimization.

```
In [ ]: def get_hilbert_shmidt_distance(gate1, gate2):
    return hilbert_dist(Qobj(gate1), Qobj(gate2))

def my_hilbert_schmidt_distance(gate1, gate2):
    return np.sqrt(1 - (np.abs(np.trace(np.conj(gate1).T @ gate2))**2) / (2*

In [ ]: print("Hilbert Schmidt Distance of CCX with itself: ", get_hilbert_shmidt_diprint("My Hilbert Schmidt Distance of CCX with itself: ", my_hilbert_schmidt

Hilbert Schmidt Distance of CCX with itself: 0.0

My Hilbert Schmidt Distance of CCX with itself: 0.0
```

Building the Circuit

We can build the circuit with 11 single qubit gates which can simply be made with qiskit's UGate. This is a generic rotation matrix of three dimensions defined by:

```
In [ ]: class SingleQubitU(Gate):
    def __init__(self, theta, phi, lam):
        super().__init__('U1', 1, [theta, phi, lam])

def __define(self):
        qc = QuantumCircuit(1)
        qc.unitary(self.to_matrix(), [0])
        self.definition = qc

def to_matrix(self):
        theta = float(self.params[0])
        phi = float(self.params[1])
        lam = float(self.params[2])
        return UGate(theta, phi, lam).to_matrix()
```

Next, we can define a generic two qubit unitary using RXX, RYY, and RZZ gates like so:

```
In [ ]: class TwoQubitU(Gate):
            def init (self, alpha1, alpha2, alpha3):
                super(). init ('U2', 2, [alpha1, alpha2, alpha3])
            def define(self):
                qc = QuantumCircuit(2)
                qc.unitary(self.to matrix(), [0, 1])
                self.definition = qc
            def to matrix(self):
                alpha1 = float(self.params[0])
                alpha2 = float(self.params[1])
                alpha3 = float(self.params[2])
                rxx gate = RXXGate(alpha1).to matrix()
                ryy gate = RYYGate(alpha2).to matrix()
                rzz gate = RZZGate(alpha3).to matrix()
                return rxx gate @ ryy gate @ rzz gate
In [ ]: class ParamVectorItterator:
            def __init__(self, param_vector):
```

```
In []: class ParamVectorItterator:
    def __init__(self, param_vector):
        self.param_vector = param_vector
        self.index = 0

    def __iter__(self):
        return self

    def __next__(self):
        if self.index < len(self.param_vector):
            start = self.index
        end = self.index + 3
            params = self.param_vector[start:end]
        self.index += 3
        return params
    else:
        raise StopIteration</pre>
```

From the paper, we know its possible to build a generic gate with 4 two qubit unitaries in the order $U_{AB}U_{BC}U_{AB}U_{AC}$. We then surround the space around the 4 unitaries with 11 single qubit unitaries. The circuit is outlined below. Each Unitary has a set of 3 rotation parameters assigned to them, allowing for a total of 45 degrees of freedom.

```
In [ ]:
        approx CCNOT qc = QuantumCircuit(3, name="Approx CCNOT")
        # Define parameters
        theta = Parameter('theta')
        phi = Parameter('phi')
        lam = Parameter('lam')
        num U1 params = 3 * 11
        num U2 params = 3 * 4
        pU1 = ParameterVector('pU1', num U1 params)
        pU1 itter = ParamVectorItterator(pU1)
        pU2 = ParameterVector('pU2', num U2 params)
        pU2 itter = ParamVectorItterator(pU2)
        # Create the circuit
        approx CCNOT qc.append(SingleQubitU(*next(pU1 itter)), [0])
        approx CCNOT qc.append(SingleQubitU(*next(pU1 itter)), [1])
        approx CCNOT qc.append(SingleQubitU(*next(pU1 itter)), [2])
        approx CCNOT qc.append(TwoQubitU(*next(pU2 itter)), [0, 1])
        approx CCNOT qc.append(SingleQubitU(*next(pU1 itter)), [1])
        approx CCNOT qc.append(SingleQubitU(*next(pU1 itter)), [0])
        approx CCNOT qc.append(TwoQubitU(*next(pU2 itter)), [1, 2])
        approx CCNOT qc.append(SingleQubitU(*next(pU1 itter)), [1])
        approx CCNOT qc.append(TwoQubitU(*next(pU2 itter)), [0, 1])
        approx CCNOT qc.append(SingleQubitU(*next(pU1 itter)), [0])
        approx_CCNOT_qc.append(SingleQubitU(*next(pU1_itter)), [1])
        approx CCNOT qc.append(SingleQubitU(*next(pU1 itter)), [2])
        approx CCNOT qc.append(TwoQubitU(*next(pU2 itter)), [0, 2])
        approx CCNOT qc.append(SingleQubitU(*next(pU1 itter)), [0])
        approx CCNOT qc.append(SingleQubitU(*next(pU1 itter)), [2])
        approx CCNOT qc.draw(output='mpl')
```

Finding a Solution Using Swarm Optimization

We need to find a set of parameters that will closely approximate a Toffoli using this circuit. An algorithm I've chosen to use is Swarm Optimization. A detailed description of the algorithm can be found here: https://machinelearningmastery.com/a-gentle-introduction-to-particle-swarm-optimization/

In a nutshell, it uses a randomly distributed amount of points that query the function. They all move about the inout space and have the ability to 'talk' to eachother, where if one particle finds a global minimum, it'll tell the rest. This causes nearby particles to 'swarm' towards it. The grouped up particles will repeatedly swarm about the current global minimum until they unconver an even smaller minimum. Then the process is repeated.

```
In [ ]: def opt_func(vals):
    distances = []
    for p in vals:
        # Get the circuit
        bound_approx_CCNOT = approx_CCNOT_qc.bind_parameters({pU1: p[:num_U1])

        # Get the matrix
        approx_CCNOT_matrix = Operator(bound_approx_CCNOT).data

        # Get the distance
        distances.append(my_hilbert_schmidt_distance(ccx_gate, approx_CCNOT_return distances)
```

Here I use the opt_func defined above and run swarm optimization using the python library Pyswarms. I've choesn my c1 parameter to be 0.5 and my c2 parameter to be 0.3. The algorithm contains 200 particles and is set to run for 2500 iterations. I had all the variables bounded between 0 and \$2\pi and they all started at random values.

```
In []: options = {'c1': 0.5, 'c2': 0.3, 'w':0.9}
bounds = (np.repeat(0, num_U1_params + num_U2_params), np.repeat(2*np.pi, nu
    optimizer = ps.single.GlobalBestPSO(n_particles=200, dimensions=num_U1_param
    cost, pos = optimizer.optimize(opt_func, iters=2500)

print("Total cost: ", cost)
    print("Best position: ", pos)
```

```
2023-02-23 17:31:48,913 - pyswarms.single.global best - INFO - Optimize for
        2500 iters with {'c1': 0.5, 'c2': 0.3, 'w': 0.9}
        pyswarms.single.global best: 100%| 2500/2500, best_cost=0.429
        2023-02-23 17:52:48,688 - pyswarms.single.global best - INFO - Optimization
        finished | best cost: 0.4287530618177782, best pos: [3.2881299 3.99184176
        3.18553378 3.2863268 1.47877481 5.09025655
         2.06475121 2.60927009 3.17647204 2.59969531 3.36538605 3.78667736
         2.66786559 2.8671362 1.69989823 2.57387439 1.70459726 2.55508443
         2.32916717 4.76582611 2.1363075 3.41773472 1.99808937 2.85485426
         3.51766326 2.50742741 3.89748721 2.82860762 4.14244896 3.91760327
         1.92736293 2.2492523 3.38994099 1.57787831 1.57906084 4.01130051
         4.89219643 1.63048575 4.10654436 4.73169744 1.55157382 3.99735117
         4.76154822 1.95726347 4.46895444]
        Total cost: 0.4287530618177782
        Best position: [3.2881299 3.99184176 3.18553378 3.2863268 1.47877481 5.0
        9025655
         2.06475121 2.60927009 3.17647204 2.59969531 3.36538605 3.78667736
         2.66786559 2.8671362 1.69989823 2.57387439 1.70459726 2.55508443
         2.32916717 4.76582611 2.1363075 3.41773472 1.99808937 2.85485426
         3.51766326 2.50742741 3.89748721 2.82860762 4.14244896 3.91760327
         1.92736293 2.2492523 3.38994099 1.57787831 1.57906084 4.01130051
         4.89219643 1.63048575 4.10654436 4.73169744 1.55157382 3.99735117
         4.76154822 1.95726347 4.468954441
In [ ]: # Saving the best position thus far
        best pos thus far = pos
```

Results

As we can see, the swarm optimization did quite well. I was able to achieve a HS distance of 0.428 - which is relatively close to the accepted minimum of ≈ 0.38 . Let's take a look at the output matrix.

```
In [ ]: def pos to matrix(pos):
            bound approx CCNOT = approx CCNOT qc.bind parameters({pU1: pos[:num U1 p
            approx CCNOT matrix = Operator(bound approx CCNOT).data
            return approx CCNOT matrix
In [ ]: |array_to_latex(pos_to_matrix(best_pos thus far))
Out[]:
           0.76866 - 0.15965i 0.15426 + 0.31358i
                                                     -0.09028 - 0.18448i
                                                                          0.08586 - 0.13
           -0.2417 + 0.20675i 0.4901 + 0.12602i
                                                     0.59797 - 0.12651i
                                                                          0.09808 + 0.0
           0.21766 - 0.28419i
                               -0.42095 - 0.42157i
                                                     0.58803 + 0.15945i
                                                                           0.11423 - 0.1
          -0.01731 - 0.10988i \quad -0.06438 + 0.01535i \quad -0.07918 + 0.03198i
                                                                          0.18388 + 0.68
          0.21389 - 0.03186i
                               0.04818 + 0.33657i
                                                     0.28136 + 0.19236i
                                                                           -0.0824 + 0.0
          -0.04262 - 0.12944i 0.33495 - 0.08285i
                                                     0.05343 - 0.02007i
                                                                          -0.08735 - 0.
           0.21151 - 0.03403i
                               -0.06794 - 0.14012i
                                                     0.22197 - 0.10344i
                                                                          -0.326 + 0.46
           0.13403 - 0.11313i 0.02965 - 0.05196i
                                                     0.15836 - 0.03555i
                                                                          0.22175 + 0.11
```

As we can see, this matrix is quite good. All of the positions where we expect to see 1s are values very close to such.

Attempt at Further Optimization

This matrix is quite good. However, we could optimize it to get a bit closer.

To start, lets consider the imaginary version of the Hilbert Schmidt Distance; which is of course 2-dimentional

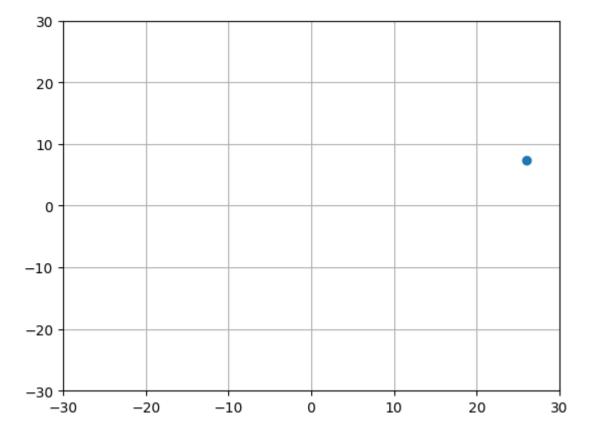
```
In [ ]: qutip_hs_dist = get_hilbert_shmidt_distance(ccx_gate, Operator(bound_approx_print(qutip_hs_dist)
```

(25.981858991915477+7.390696236864459j)

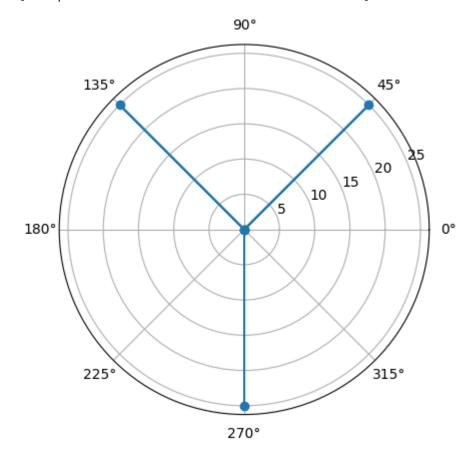
Now, lets plot the HS distance on a polar plot centered around zero

```
In [ ]: plt.scatter([qutip_hs_dist.real], [qutip_hs_dist.imag])
    plt.grid()
    plt.xlim([-30, 30])
    plt.ylim([-30, 30])
```

```
Out[]: (-30.0, 30.0)
```



Lets choose 3 points we can optimize around. Here they are at pi/4, 3pi/4 and 3pi/2



If we can possibly optimize a set of matrices centered around *different* points. Then we can use approximate computation (similar to QUEST) by calculating an average matrix of all of them.

Lets define a new optimization function that takes in a shifted value from the HS distance. Then we perform swam optimization once more on each of these shifted distances

```
In [ ]: def swarm(center_point, num_particles=100, num_iters=1000):
    options = {'c1': 0.5, 'c2': 0.3, 'w':0.9}
    bounds = (np.repeat(0, num_U1_params + num_U2_params), np.repeat(2*np.pi
    optimizer = ps.single.GlobalBestPSO(n_particles=num_particles, dimension
    cost, pos = optimizer.optimize(opt_func_shift, iters=num_iters, center=c
    return cost, pos
```

```
In []: def opt_func_shift(vals, center):
    distances = []
    for p in vals:
        # Get the circuit
        bound_approx_CCNOT = approx_CCNOT_qc.bind_parameters({pU1: p[:num_U1]})

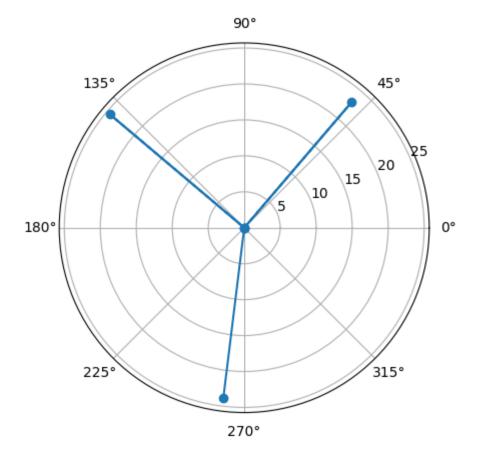
        # Get the matrix
        approx_CCNOT_matrix = Operator(bound_approx_CCNOT).data

        # Get the distance
        distances.append(get_hilbert_shmidt_distance(ccx_gate, approx_CCNOT_
        return distances + center

In []: cost_pos1, pos_pos1 = swarm(opt_point1, num_particles=100, num_iters=1000)
        cost_pos2, pos_pos2 = swarm(opt_point2, num_particles=100, num_iters=1000)
        cost_pos3, pos_pos3 = swarm(opt_point3, num_particles=100, num_iters=1000)
```

```
1000 iters with {'c1': 0.5, 'c2': 0.3, 'w': 0.9}
        pyswarms.single.global best: 100%| | 1000/1000, best cost=14.9+17.5
        2023-02-24 19:04:25,041 - pyswarms.single.global best - INFO - Optimization
        finished | best cost: (14.947570760863105+17.49957230658889j), best pos:
        [4.94852239 5.31990243 2.72016298 2.52436342 5.07355072 3.8872982
         2.90433733 1.47252178 4.87271872 1.472074 3.29548535 1.20690037
         3.28364791 4.07272721 3.05815181 5.13989982 3.56239027 2.45110943
         2.81320373 3.47888178 2.00305014 2.99351045 2.38845607 3.27279178
         3.76155527 1.73367278 3.60487945 1.57368081 3.47171195 4.63285325
         3.64088159 1.90793813 4.07857064 3.84096104 5.31429011 2.7523648
         5.35741858 2.64941561 3.77728354 3.41822824 0.33558311 2.59505671
         3.40351711 2.26134192 2.91022288]
        2023-02-24 19:04:25,051 - pyswarms.single.global best - INFO - Optimize for
        1000 iters with {'c1': 0.5, 'c2': 0.3, 'w': 0.9}
        pyswarms.single.global best: 100%| | 1000/1000, best_cost=-18.7+15.
        8j
        2023-02-24 19:17:08,493 - pyswarms.single.global best - INFO - Optimization
        finished | best cost: (-18.70159143943443+15.803896261701501j), best pos:
        [3.65813699 2.20360965 4.96830455 0.22032852 2.21555011 1.12597795
         2.59663447 0.8376655 2.38897694 3.85048812 1.92046155 1.29820114
         3.53804372 3.06051318 3.47328148 3.41827793 1.93526526 3.49683556
         3.79325234 4.09740866 4.13758411 6.13515788 2.91750183 2.85017197
         2.30059826 3.17825267 3.44485304 3.73410987 2.17827143 3.94234458
         4.50626074 3.55246323 4.83272395 1.63899373 1.38762747 4.22771967
         1.94659978 2.78654343 3.02964671 1.91887559 4.56346941 1.55961505
         3.67840085 0.94189995 3.06790657]
        2023-02-24 19:17:08,506 - pyswarms.single.global best - INFO - Optimize for
        1000 iters with {'c1': 0.5, 'c2': 0.3, 'w': 0.9}
        pyswarms.single.global best: 100%| | 1000/1000, best cost=-2.91-23.
        2023-02-24 19:30:02,637 - pyswarms.single.global best - INFO - Optimization
        finished | best cost: (-2.910532419972098-23.731059806466718j), best pos:
        [3.31937089 4.08372469 4.93494652 3.10549009 3.0658602 2.51631658
         4.61207406 3.31491016 3.21046124 4.28797036 3.47631791 3.28448812
         2.85181143 2.69417498 3.8968485 3.30453134 4.35808709 3.72272129
         4.25351947 2.6790646 3.29649022 2.02026226 3.15979941 3.41766571
         1.26042811 3.30254734 1.38923825 2.27978336 3.12086983 3.69036325
         2.66367921 2.46728138 5.18724274 3.17041132 2.76535835 3.39010443
         2.95430432 2.52661284 3.84968976 3.68019831 3.33942254 3.02380828
         3.61595185 3.42158961 3.57915215]
In [ ]: | tot cost pos1 = cost pos1-opt point1
        tot cost pos2 = cost pos2-opt point2
        tot cost pos3 = cost pos3-opt point3
        print(tot_cost_pos1)
        (-2.730098768800584-0.17809722307479348j)
In [ ]: #plt.polar([0, np.angle(cost pos1)], [0, np.abs(cost pos1)], marker='o')
        plt.polar([0, np.angle(cost pos1), 0, np.angle(cost pos2),0,np.angle(cost po
Out[ ]: [<matplotlib.lines.Line2D at 0x7f21175c9990>]
```

2023-02-24 18:51:38,870 - pyswarms.single.global best - INFO - Optimize for



```
array_to_latex(pos_to_matrix(pos_pos1))
Out[]:
           0.67054 - 0.04844i
                                 0.19283 - 0.06341i
                                                       -0.24934 - 0.23378i
                                                                             0.24221 - 0.0
           -0.40004 - 0.04437i
                                 0.77973 - 0.18047i
                                                       -0.12443 - 0.14944i
                                                                             -0.10744+0.
           0.19655 - 0.43396i
                                 0.12752 - 0.27401i
                                                       0.49702 - 0.07831i
                                                                             0.18275 + 0.0
           -0.11847 + 0.10084i
                                 0.26484 + 0.03139i
                                                       -0.04296 + 0.17028i
                                                                              0.11337 - 0.1
           -0.26075 - 0.07888i
                                 -0.15578 + 0.12252i
                                                       -0.27248 + 0.37328i
                                                                             0.20961 - 0.0
            -0.02643 - 0.07i
                                   0.01298 + 0.25i
                                                       0.15581 + 0.08201i
                                                                              0.07178 + 0.1
           0.18726 + 0.04434i
                                                                             -0.04911 + 0.
                                  0.20628 + 0.1008i
                                                       -0.52155 + 0.17461i
           -0.13293 + 0.01902i
                                 0.00781 + 0.03246i
                                                       -0.01081 + 0.11897i
                                                                             0.62984 + 0.4
```

In []: array_to_latex(pos_to_matrix(pos_pos2))

```
Out[]:
           0.55903 + 0.26577i
                                 0.30404 - 0.21834i
                                                       0.01134 + 0.13835i
                                                                            -0.02806 - 0.
           -0.42695 - 0.38775i
                                                                             0.04828 - 0.0
                                 0.22969 + 0.47832i
                                                      -0.02469 + 0.11892i
           0.01395 + 0.02364i
                                -0.21711 + 0.02924i
                                                                              0.12834 - 0.
                                                       0.38826 + 0.43931i
            0.0936 - 0.05242i
                                 0.08926 - 0.1318i
                                                       -0.0458 - 0.422i
                                                                             0.40988 + 0.4
           -0.37095 - 0.18335i
                                -0.07492 - 0.62335i
                                                       0.15519 - 0.04476i
                                                                            -0.03532 - 0.
           -0.18978 - 0.24113i
                                 0.22541 - 0.22884i
                                                       -0.073 + 0.00269i
                                                                            -0.06708 - 0.
           -0.01082 - 0.0346i
                                 0.05026 - 0.04096i
                                                      -0.23382 - 0.48438i
                                                                           -0.21016 - 0.
          -0.01297 + 0.07135i
                                 -0.0445 + 0.03837i
                                                      -0.03321 - 0.34674i
                                                                             0.14225 - 0.1
In [ ]: | array to latex(pos to matrix(pos pos3))
Out[]:
           0.59526 - 0.47335i
                                -0.10777 - 0.20738i
                                                       0.0361 + 0.26107i
                                                                             0.20596 - 0.1
          -0.03202 - 0.01246i
                                 0.49957 - 0.04574i
                                                       0.14781 + 0.21945i
                                                                            -0.06865+0.
           0.02362 + 0.29389i
                                -0.08189 + 0.14434i
                                                       0.48692 - 0.54809i
                                                                             0.1847 + 0.03
          -0.13827 + 0.08496i
                                 0.01722 + 0.18098i
                                                      -0.09977 + 0.11849i
                                                                             0.06262 - 0.0
           0.14571 + 0.48578i
                                -0.24578 - 0.12794i
                                                                             0.01237 - 0.1
                                                       0.0598 + 0.41276i
           0.09467 - 0.03456i
                                 0.17666 + 0.66544i
                                                      -0.00122 + 0.16053i
                                                                             0.24408 + 0.2
           -0.12731 - 0.04825i
                                 -0.0089 - 0.16755i
                                                      -0.09172 + 0.07995i
                                                                            -0.11067 + 0.
           -0.12263 - 0.0788i
                                -0.22513 + 0.05904i \quad -0.26769 + 0.11342i
                                                                             0.28204 + 0.2
        average mat = (pos\ to\ matrix(pos\ pos1)\ +\ pos\ to\ matrix(pos\ pos2)\ +\ pos\ to\ ma
In [ ]:
        array to latex(average mat)
Out[]:
           0.60827 - 0.08534i
                                 0.1297 - 0.16305i
                                                       -0.0673 + 0.05521i
                                                                             0.14003 - 0.1
           -0.28634 - 0.14819i
                                  0.503 + 0.08404i
                                                      -0.00043 + 0.06297i
                                                                            -0.04261+0.
           0.07804 - 0.03881i
                                -0.05716 - 0.03347i
                                                       0.4574 - 0.06236i
                                                                             0.16526 - 0.0
           -0.05438 + 0.04446i
                                 0.12377 + 0.02686i
                                                      -0.06284 - 0.04441i
                                                                             0.19529 - 0.1
            -0.162 + 0.07452i
                                -0.15883 - 0.20959i
                                                                             0.06222 - 0.1
                                                     -0.01916 + 0.24709i
           -0.04052 - 0.11523i
                                 0.13835 + 0.22887i
                                                       0.0272 + 0.08174i
                                                                             0.08293 + 0.1
           0.01638 - 0.01283i
                                 0.08255 - 0.0359i
                                                       -0.28236 - 0.0766i
                                                                            -0.12331 - 0.
          -0.08951 + 0.00386i
                                -0.08727 + 0.04329i
                                                      -0.1039 - 0.03812i
                                                                             0.35137 + 0.1
In [ ]: get hilbert shmidt distance(ccx gate, average mat)
Out[]: (0.9684075801453074-0.3784580050822781j)
In [ ]: my_hilbert_schmidt_distance(ccx_gate, average_mat)
Out[]: 0.8768918012485036
In [ ]:
```