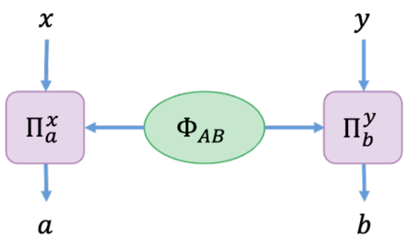
Variational Quantum Optimization (VQO) of CHSH Violation

This notebook demonstrates how quantum machine learning can be applied to train a quantum circuit to violate the Bell inequality.



- $x, y \in \{0, 1\}$ and $a, b \in \{-1, 1\}$.
- Local qubit measurements Π_a^x and Π_b^y are projective.
- State preparation Φ^{AB} is a static, bipartite quantum state.

$$I_{CHSH} = \sum_{x,y\in\{0,1\}} (-1)^{x\wedge y}\langle A_x B_y\rangle \leq 2$$

Goal: Find state preparation and measurements that maximally violate the CHSH inequality.

Requirements

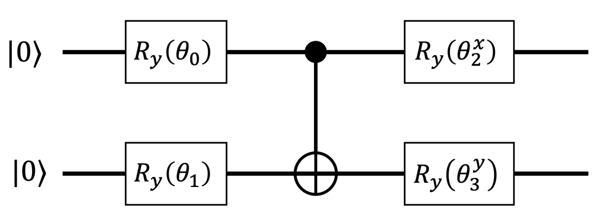
This code requires the `pennylane` and `matplotlib` python libraries.

In [1]:

```python
# quantum machine learning framework
import pennylane as qml

# numpy extension for pennylane
from pennylane import numpy as np

# plotting utility
import matplotlib.pyplot as plt
```

CHSH Ansatz

We consider a simple ansatz circuit $U^{AB}_{CHSH}(\vec{\theta})$ for the CHSH scenario.



- **State Preparation:** local qubit rotations about the y-axis followed by a CNOT gate. Can prepare any pure state in the Bell basis or omputational basis.
- **Measurement:** The computational basis is rotated about the y-axis allowing any projective measurement in the x-z-plane to be realized.

$$\begin{aligned} U_{CHSH}^{AB}(\vec{\theta})|00\rangle^{AB} &= \left(R_y^A(\theta_2)\otimes R_y^B(\theta_3)\right)U_{CNOT}^{AB}\left(R_y^A(\theta_0)\otimes R_y^B(\theta_1)\right)|00\rangle^{AB} && (1)\\ &= \left(R_y^A(\theta_2)\otimes R_y^B(\theta_3)\right)|\psi(\theta_0,\theta_1)\rangle^{AB} && (2)\\ &= |\psi_{CHSH}(\vec{\theta})\rangle^{AB} && (3)\end{aligned}$$

This ansatz parameterizes real-valued states and measurements, but is sufficient to find

In [2]:

```python
def chsh_ansatz(settings, wires):
    # state prepartion
    qml.RY(settings[0], wires=wires[0])
    qml.RY(settings[1], wires=wires[1])
    qml.CNOT(wires=wires[0:2])

    # measurement basis rotations
    qml.RY(settings[2], wires=wires[0])
    qml.RY(settings[3], wires=wires[1])
```

Ansatz Parameterization

The CHSH scenario has a static state preparation and two inputs, $x, y \in \{0, 1\}$ that select local measurement bases.

We organize our settings into preparation and measurement settings:

$$\vec{\theta} = (\{\theta\}^P, \{\theta\}^M) = \left([\theta_0, \theta_1], \begin{bmatrix} \theta_2^{x=0} & \theta_2^{x=1} \\ \theta_3^{x=0} & \theta_3^{x=1} \end{bmatrix}\right)$$

while $\vec{\theta}_{x,y} = [\theta_0, \theta_1, \theta_2^x, \theta_3^y]$. We now write a function create randomized initial parameters.

In [3]:

```python
def random_scenario_settings():
    preparation_settings = np.random.random(2)
    measurement_settings = np.random.random((2,2))

    return [preparation_settings, measurement_settings]

random_scenario_settings()
```

Out[3]:

```
[tensor([0.37895832, 0.00818022], requires_grad=True),
 tensor([[0.14476653, 0.61528113],
         [0.4289039 , 0.1094481 ]], requires_grad=True)]
```

PennyLane Devices

PennyLane uses a `Device` class to model quantum hardware.

- Devices can be either a classical simulator or quantum hardware.
- Devices can run locally on your laptop or executed remotely by a third party.

For this demo, we use the default state-vector simulator. We only need two qubits (`wires`). This device will numerically evaluate the quantum circuit expectations rather than constructing a distribution through sampling.

In [4]:
```
chsh_dev = qml.device("default.qubit", wires=[0,1])
```

PennyLane QNodes

A quantum node (`QNode`) class describes a quantum circuit run by a particular device. The `QNode` is a differentiable function with customizeable optimizer interfaces and gradient methods. A qnode

The `@qml.qnode` decorator specifies that the `chsh_dev` device is used to execute the `chsh_correlator` function.

The CHSH correlator extends our ansatz with a joint observable expectation

$$\begin{aligned}
\langle A_x B_y\rangle(\vec{\theta}_{x,y}) &= \langle\psi(\theta_0,\theta_1)|A_x(\theta_2)B_y(\theta_3)|\psi(\theta_0,\theta_1)\rangle && (4)\\
&= \sum_{i,j\in\{0,1\}}(-1)^{i\oplus j}\left|\langle ij|R_y^A(\theta_2)\otimes R_y^B(\theta_3)|\psi(\theta_0,\theta_1)\rangle^{AB}\right|^2 && (5)\\
&= \sum_{i,j\in\{0,1\}}(-1)^{i\oplus j}\left|\langle ij|U_{CHSH}^{AB}(\vec{\theta}_{x,y})|00\rangle^{AB}\right|^2 && (6)
\end{aligned}$$

Here $|ij\rangle$ is the computational basis. The labels x and y on the observables correspond to different parameter vectors $\vec{\theta}_{x,y}$

In [5]:
```
@qml.qnode(chsh_dev)
def chsh_correlator(settings):
    wires = chsh_dev.wires
    chsh_ansatz(settings, wires)

    # computational basis measurement
    return qml.expval(
        qml.PauliZ(wires[0]) @ qml.PauliZ(wires[1])
    )
```

Drawing the Ansatz Circuit

In [6]:
```
chsh_correlator([0,0,0,0])
print(chsh_correlator.draw())
```

```
0: ──RY(0)──╭C──RY(0)──╭┤ ⟨Z ⊗ Z⟩
1: ──RY(0)──╰X──RY(0)──╰┤ ⟨Z ⊗ Z⟩
```

Evaluating a QNode

In [7]:

```
print("00 prep and ZZ meas : ", chsh_correlator([0,0,0,0]))
```

```
00 prep and ZZ meas :  1.0
```

In [8]:

```
print("01 prep and ZZ meas : ", chsh_correlator([0,np.pi,0,0]))
```

```
01 prep and ZZ meas :  -1.0
```

In [9]:

```
print("00 prep and XX meas : ", chsh_correlator([0,0,-np.pi/2,-np.pi/2]))
```

```
00 prep and XX meas :  0.0
```

In [10]:

```
print("bell prep and ZZ meas : ", chsh_correlator([np.pi/2,0,0,0]))
```

```
bell prep and ZZ meas :  1.0
```

In [11]:

```
print("bell prep and XX meas : ", chsh_correlator([np.pi/2,0,-np.pi/2,-np.pi/
```

```
bell prep and XX meas :  0.9999999999999998
```

In [12]:

```
print("bell prep and ZX meas : ", chsh_correlator([np.pi/2,0,0,-np.pi/2]))
```

```
bell prep and ZX meas :  2.220446049250313e-16
```

The CHSH Cost Function

The CHSH inequality is expressed as:

$$I_{CHSH}(\vec{\theta}) = \sum_{x,y\in\{0,1\}} (-1)^{x\wedge y}\langle A_x B_y\rangle(\vec{\theta}_{x,y})$$

The corresponding cost function is expressed as:

$$\text{Cost}(\vec{\theta}) = -I_{CHSH}(\vec{\theta})$$

In [13]:

```
def chsh_cost(scenario_settings):

    score = 0
    for x, y in [[0,0],[0,1],[1,0],[1,1]]:
        # construct the settings for inputs `x` and `y`
        qnode_settings = [
            *scenario_settings[0],
            scenario_settings[1][0,x],
            scenario_settings[1][1,y]
        ]

        # evaluate the `chsh_correlator` qnode
        score += (-1)**(x * y) * chsh_correlator(qnode_settings)

    # invert score because cost is minimized
    return -(score)
```

Gradient Descent

Our goal is to find $\arg\min_{\vec{\theta}} \text{Cost}(\vec{\theta})$ using automatic differentiation and gradient descent. This minimization problem is equivalent to maximizing the CHSH violation.

$$\begin{aligned} \vec{\theta}' &= \vec{\theta} - \eta \nabla_{\vec{\theta}} \text{Cost}(\vec{\theta}) && (7) \\ &= \vec{\theta} + \eta \nabla_{\vec{\theta}} I_{CHSH}(\vec{\theta}) && (8) \end{aligned}$$

PennyLane handles the automatic differentiation of the `chsh_correlator` QNode. We add a loop that iteratively computes the gradient and updates the settings. Each step in this training procedure is called an epoch.

In [14]:

```
def gradient_descent(cost, settings, step_size=0.1, num_steps=20):
    # optimizer work horse
    opt = qml.GradientDescentOptimizer(stepsize=step_size)

    scores = []
    settings_list = []
    for i in range(num_steps):
        # log data
        score = -(cost(settings))
        scores.append(score)
        settings_list.append(settings)

        # print progress
        if i % 5 == 0:
            print("iteration : ", i, ", score : ", score)

        # update settings using gradient evaluated at `settings`
        settings = opt.step(cost, settings)

    # log data for final score and settings
    final_score = -(cost(settings))
    scores.append(final_score)
    settings_list.append(settings)

    # find the maximum value and optimal settings
    max_score = max(scores)
    max_id = scores.index(max_score)
    opt_settings = settings_list[max_id]

    return {
        "max_score" : max_score,
        "opt_settings" : opt_settings,
        "max_id" : max_id,
        "samples" : range(num_steps + 1),
        "scores" : scores,
        "settings" : settings_list
    }
```

VQO of a Maximally Nonlocal CHSH Protocol

In [15]:

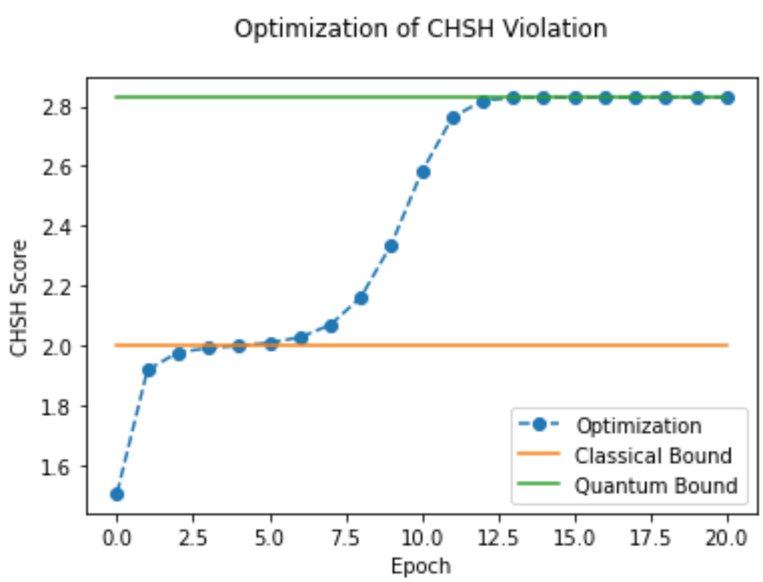
```
%%time

# initialize random parameters
init_settings = random_scenario_settings()
print("initial settings :\n", init_settings, "\n")

opt_dict = gradient_descent(chsh_cost, init_settings, step_size=0.5);

print("\nmax score : ", opt_dict["max_score"])
print("optimal settings : ", opt_dict["opt_settings"], "\n")
print("theoretical max : ", 2 * np.sqrt(2), "\n")
```

```
initial settings :
 [tensor([0.96123244, 0.55235034], requires_grad=True), tensor([[0.37514297,
0.50044924],
```

```
        [0.29133242, 0.46641267]], requires_grad=True)]

iteration :  0 , score :  1.5088222141327297
iteration :  5 , score :  2.010436716885594
iteration :  10 , score :  2.5808417015638088
iteration :  15 , score :  2.8284193404598703

max score :  2.828427124707118
optimal settings :  [array([ 1.57079231e+00, -1.06968197e-06]), array([[ 0.71
599797, -0.85479238],
       [-0.06939297,  1.50139766]])]

theoretical max :  2.8284271247461903

CPU times: user 436 ms, sys: 21.8 ms, total: 458 ms
Wall time: 448 ms
```

In [16]:

```
plt.plot(opt_dict["samples"], opt_dict["scores"], "o--", label="Optimization"
plt.plot(opt_dict["samples"], [2]*len(opt_dict["samples"]), label="Classical
plt.plot(opt_dict["samples"], [2*np.sqrt(2)]*len(opt_dict["samples"]), label=

plt.title("Optimization of CHSH Violation\n")
plt.ylabel("CHSH Score")
plt.xlabel("Epoch")
plt.legend()

plt.show()
```



In [ ]: