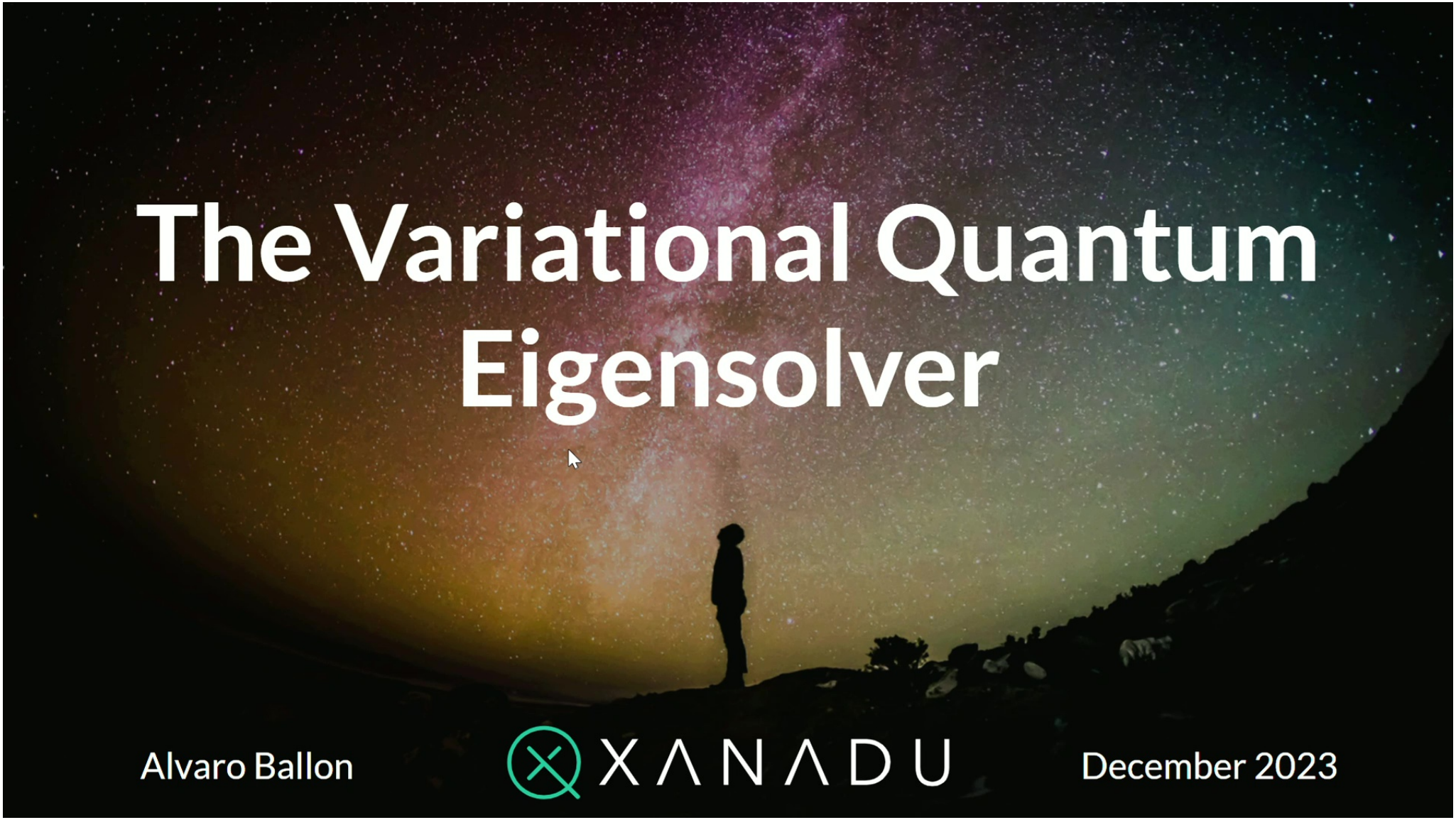
Title: Quantum Machine Learning

Speakers: Alvaro Ballon Bordo

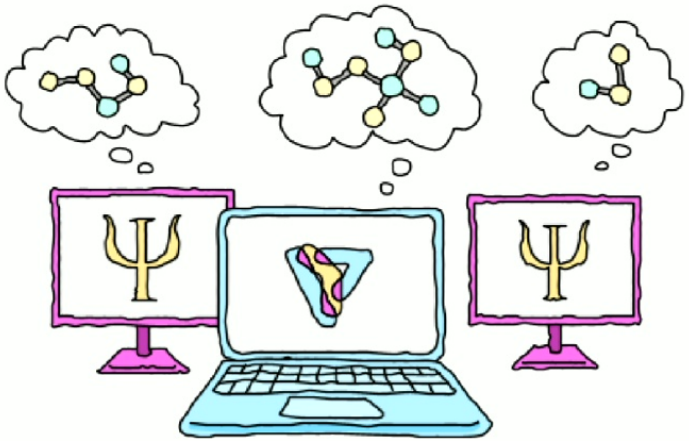
Collection: Navigating Quantum and AI Career Trajectories: A Beginnerâ€™s Mini-Course on Computational Methods and their Applications

Date: May 22, 2024 - 9:30 AM

URL: https://pirsa.org/24050084


The Variational Quantum Eigensolver
Alvaro Ballon
XANADU
December 2023

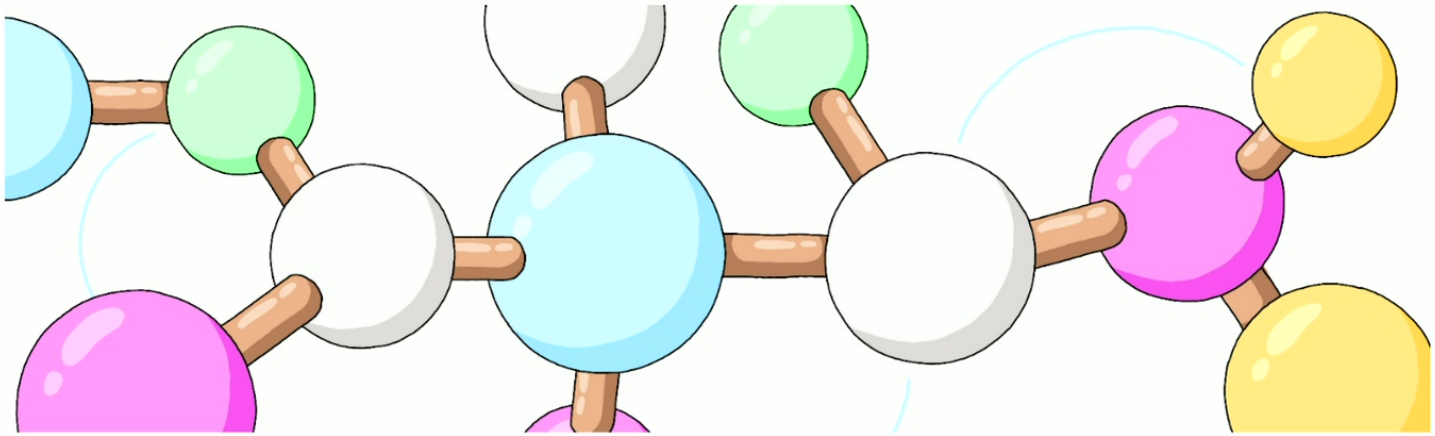
The ultimate goal of Quantum Chemistry



The dream: predict large-scale properties of matter by simulating its small scale physics.

Why? Too many applications to count. Simulating chemical reactions without going to the lab has applications in the energy, pharmaceutical, and manufacturing industries.

The challenge



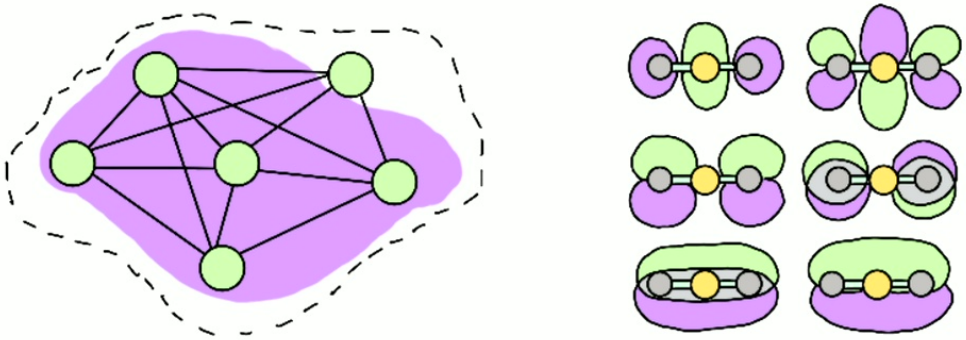
Matter is a large collection of interacting atoms, which also have nuclear and electronic substructure. Described by a Hamiltonian $\hat{H}$ which is usually large.

We need to solve Schrodinger's equation for this Hamiltonian, which is too hard!

$$\hat{H}\,\Psi(\mathbf{R},\mathbf{r}) = E\,\Psi(\mathbf{R},\mathbf{r})$$

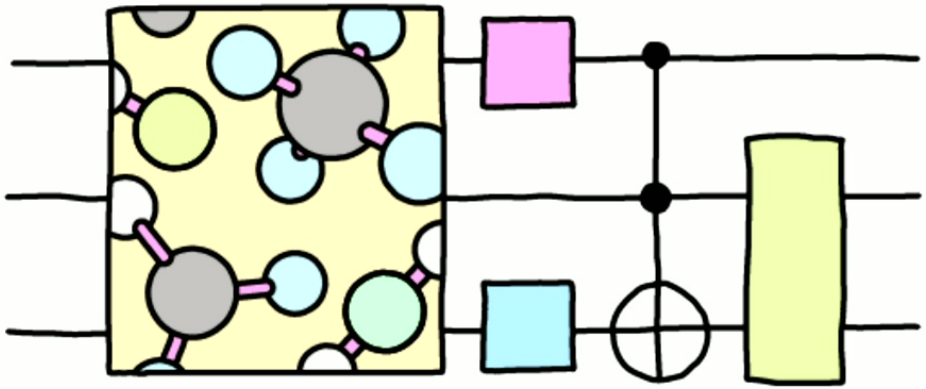
Can we try anyway?

Idea: Use an approximation, called the Hartree-Fock approximation.



Treat electrons as independent and average out effects of electrons on other electrons. Works out nicely! But for our dream applications, **we need more.**

Enter quantum computers

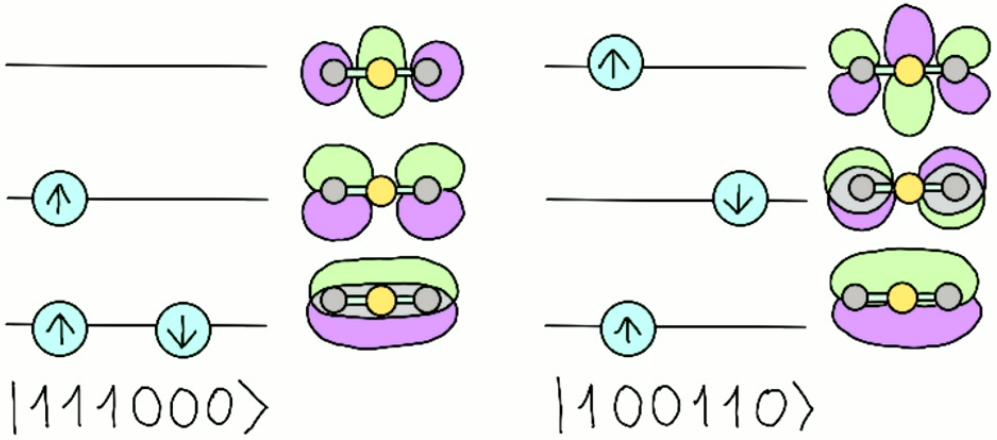


Use quantum computers to **improve on** the Hartree-Fock approximation.

These are quantum **post-Hartree Fock methods**. We will assume we know the Hartree-Fock approximated solution.

We need a way to represent molecules and Hamiltonians using qubits!

Molecule wave function as qubits



Special interest: Ground state. In the Hartree-Fock approximation, it is the Hartree-Fock state $|1,1,\ldots,1,0,0,\ldots,0\rangle$.

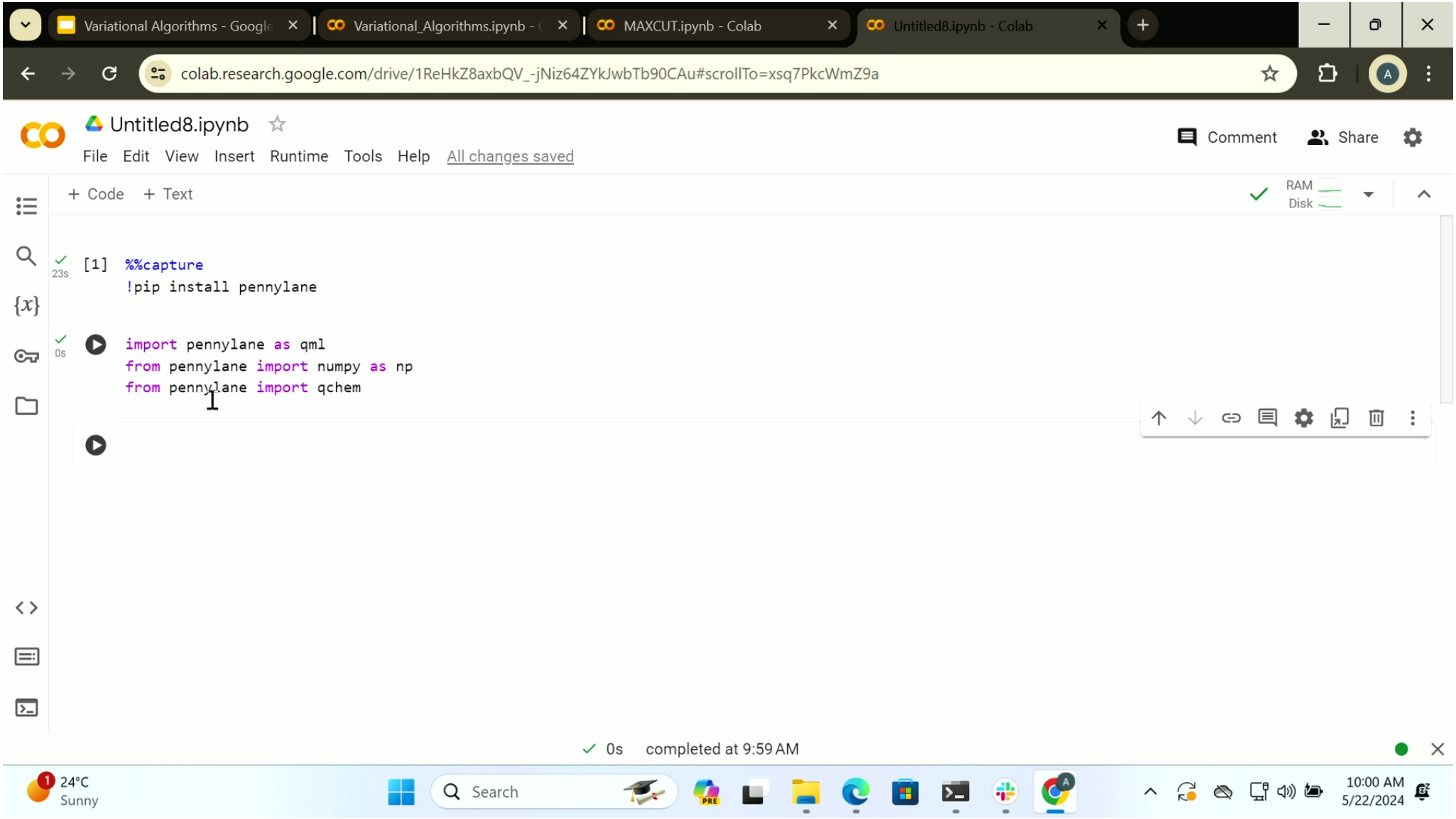
Hamiltonian as a qubit operator

$$\hat{H}\,\Psi(\mathbf{R},\mathbf{r}) = E\,\Psi(\mathbf{R},\mathbf{r})$$

$$H = \sum_{p,q} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

$$\begin{aligned} \hat{a}_p &= \tfrac{1}{2}(X_p + iY_p) \otimes Z_{p-1} \cdots \otimes Z_0 \\ \hat{a}_p^\dagger &= \tfrac{1}{2}(X_p - iY_p) \otimes Z_{p-1} \cdots \otimes Z_0 \end{aligned}$$

Overwhelmed much? PennyLane can save you all this work!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[1] %%capture
!pip install pennylane
0s
import pennylane as qml
from pennylane import numpy as np
from pennylane import qchem
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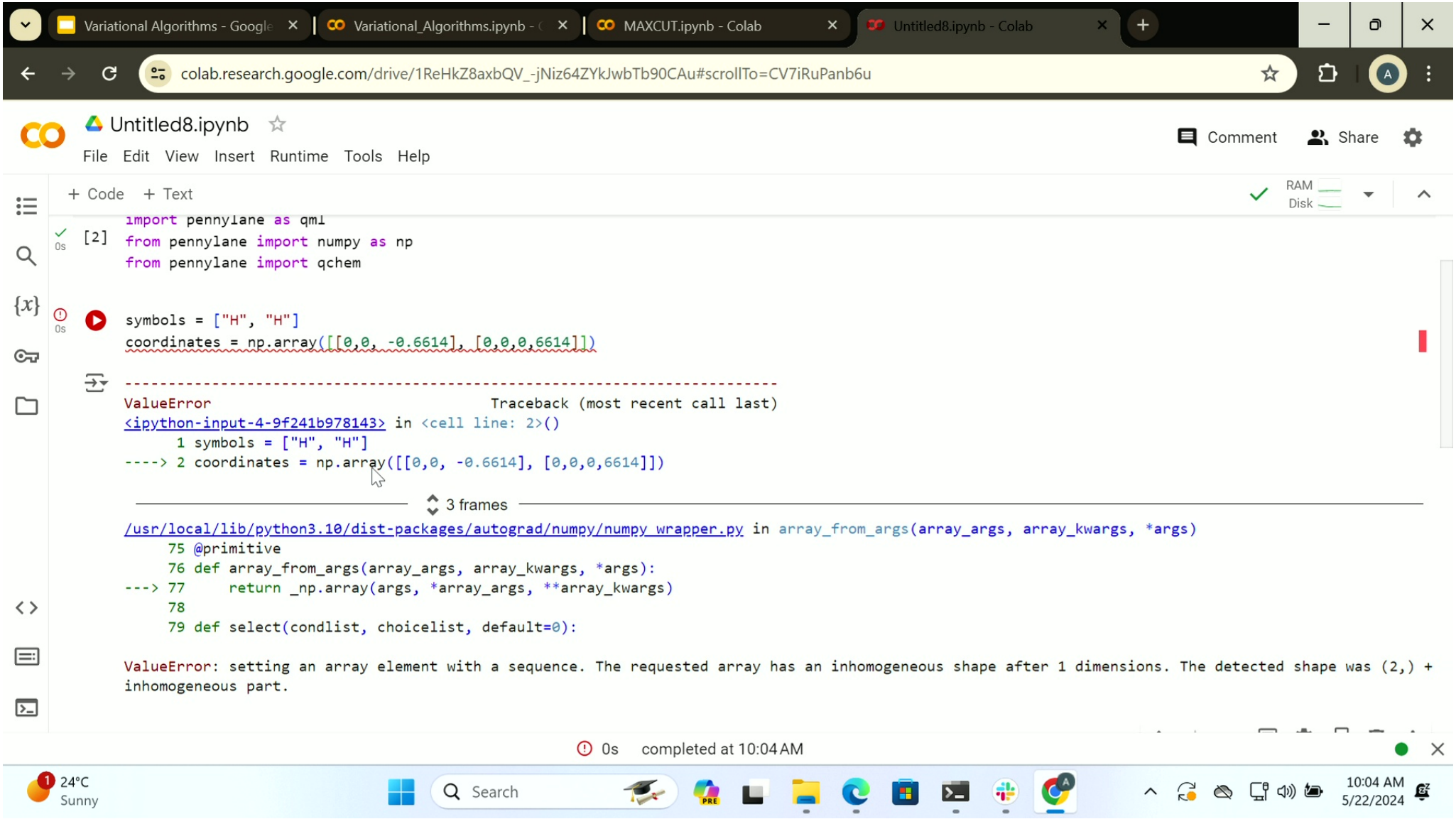
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[2]
0s
import pennylane as qml
from pennylane import numpy as np
from pennylane import qchem
symbols = ["H", "H"]
coordinates = np.array([[0,0, -0.6614], [0,0,0,6614]])
ValueError Traceback (most recent call last)
<ipython-input-4-9f241b978143> in <cell line: 2>()
1 symbols = ["H", "H"]
----> 2 coordinates = np.array([[0,0, -0.6614], [0,0,0,6614]])
3 frames
/usr/local/lib/python3.10/dist-packages/autograd/numpy/numpy_wrapper.py in array_from_args(array_args, array_kwargs, *args)
75 @primitive
76 def array_from_args(array_args, array_kwargs, *args):
---> 77 return _np.array(args, *array_args, **array_kwargs)
78
79 def select(condlist, choicelist, default=0):
ValueError: setting an array element with a sequence. The requested array has an inhomogeneous shape after 1 dimensions. The detected shape was (2,) + inhomogeneous part.
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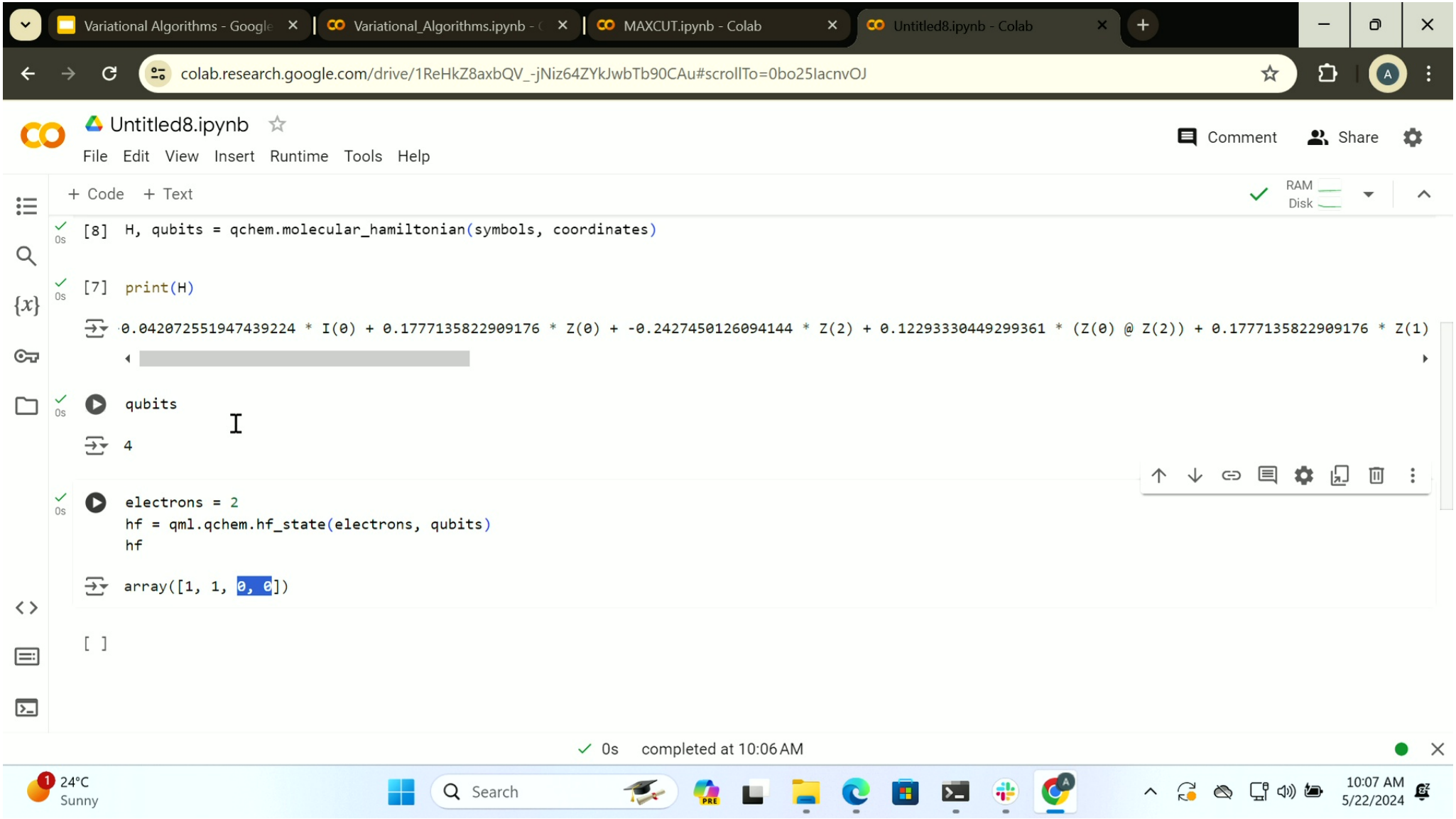
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[8] H, qubits = qchem.molecular_hamiltonian(symbols, coordinates)
0s
[7] print(H)
0s
0.042072551947439224 * I(0) + 0.1777135822909176 * Z(0) + -0.2427450126094144 * Z(2) + 0.12293330449299361 * (Z(0) @ Z(2)) + 0.1777135822909176 * Z(1)
qubits
0s
4
electrons = 2
hf = qml.qchem.hf_state(electrons, qubits)
hf
0s
array([1, 1, 0, 0])
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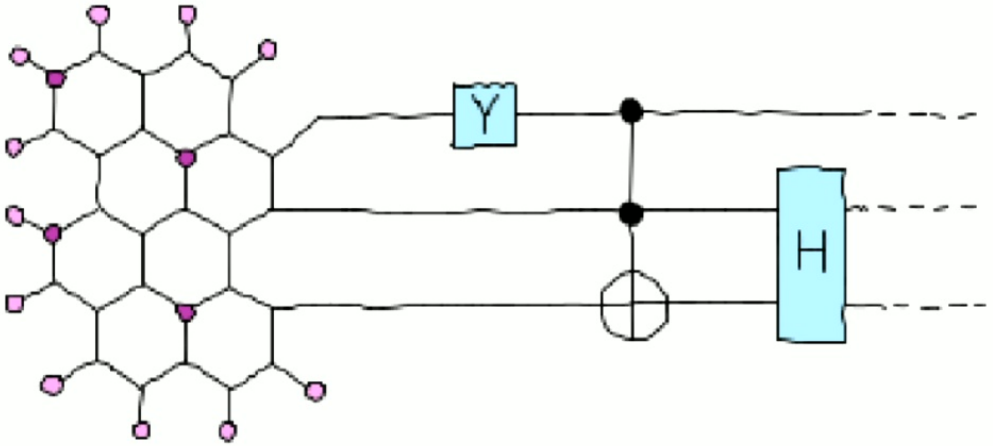
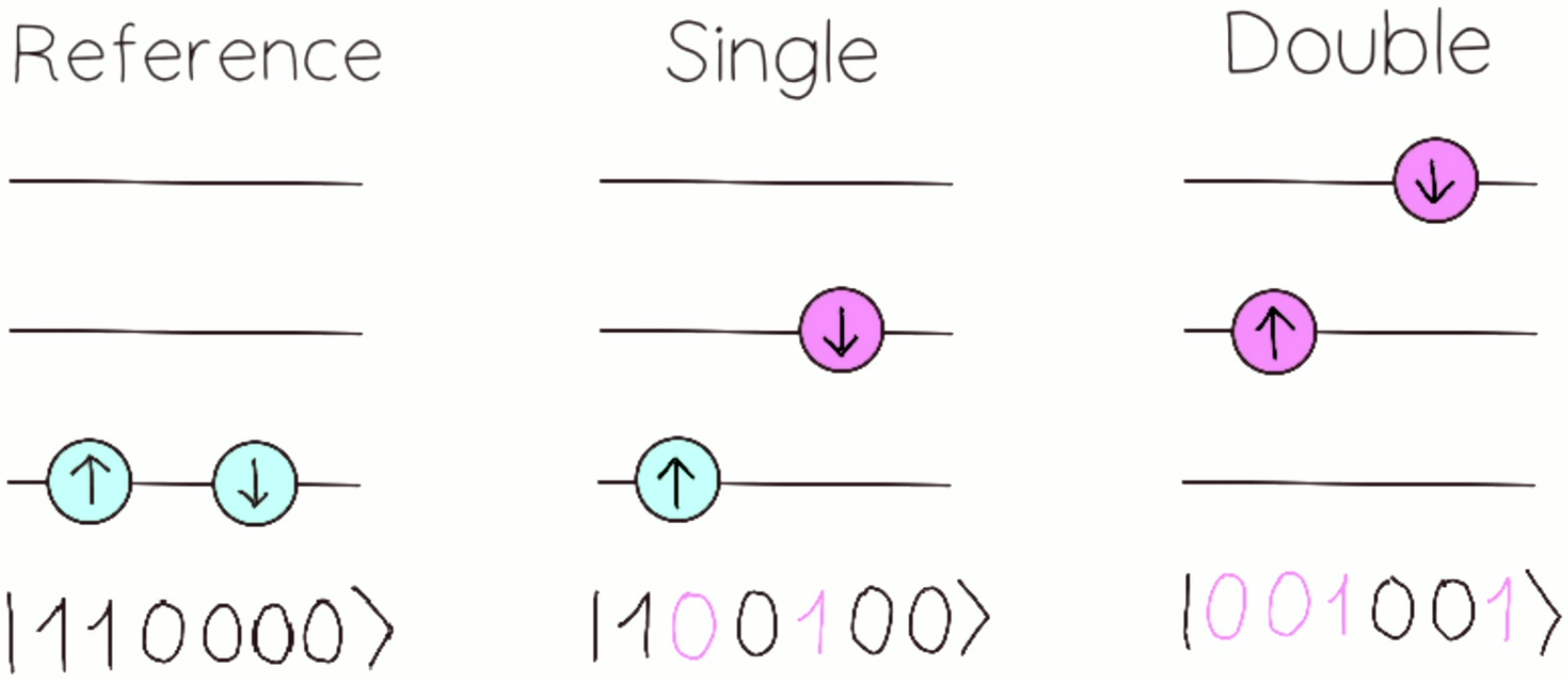
Variational Quantum Eigensolver (VQE)



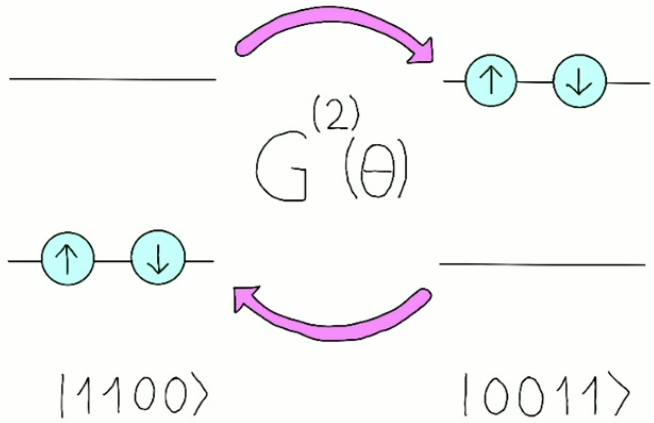
Post-Hartree Fock algorithm to find **ground state** of system described by $\hat{H}$.

1. Prepare Hartree-Fock state.
2. Create an **ansatz** which:
   a. Prepares a family of candidate ground states
   b. Measure the expectation value of the Hamiltonian
3. Optimize circuit parameters to minimize the expectation value.

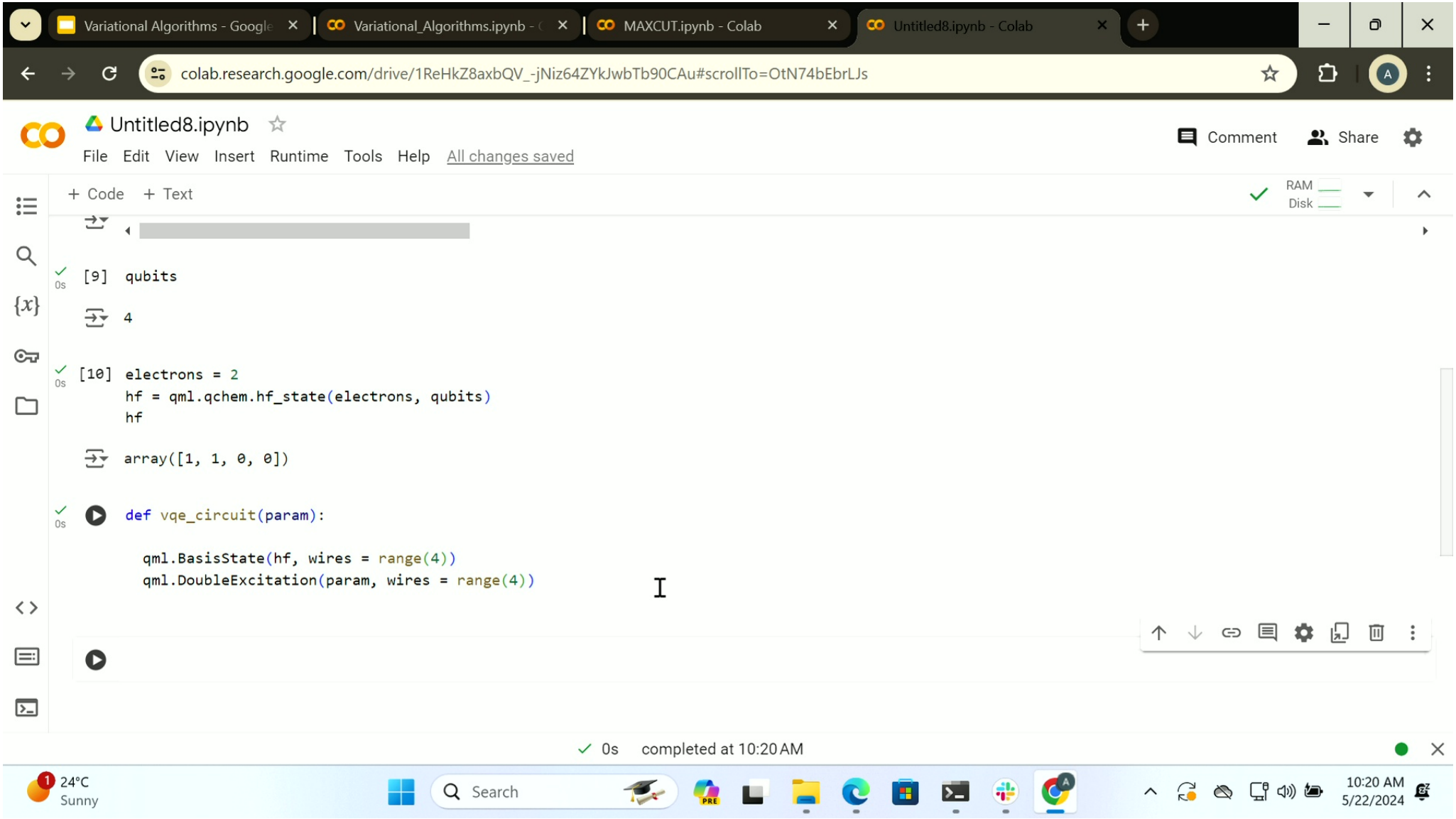
Excitation gates



Double excitation gate



$$G^{(2)}|0011\rangle = \cos(\theta/2)|0011\rangle + \sin(\theta/2)|1100\rangle$$
$$G^{(2)}|1100\rangle = \cos(\theta/2)|1100\rangle - \sin(\theta/2)|0011\rangle$$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RAM
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[9] qubits
4
[10] electrons = 2
hf = qml.qchem.hf_state(electrons, qubits)
hf
array([1, 1, 0, 0])
def vqe_circuit(param):
qml.BasisState(hf, wires = range(4))
qml.DoubleExcitation(param, wires = range(4))
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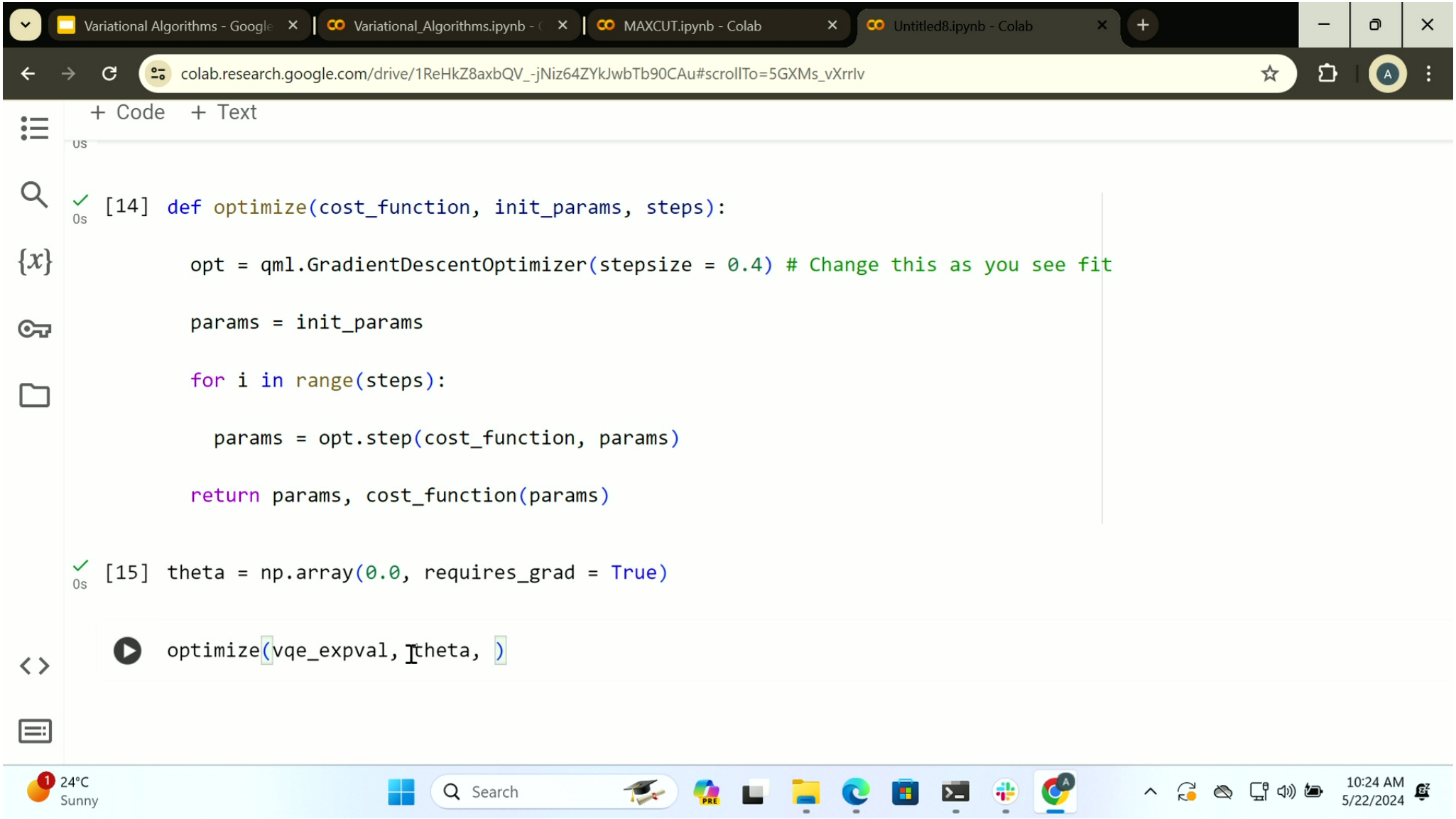
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[14] def optimize(cost_function, init_params, steps):
opt = qml.GradientDescentOptimizer(stepsize = 0.4) # Change this as you see fit
params = init_params
for i in range(steps):
params = opt.step(cost_function, params)
return params, cost_function(params)
[15] theta = np.array(0.0, requires_grad = True)
optimize(vqe_expval, theta,)
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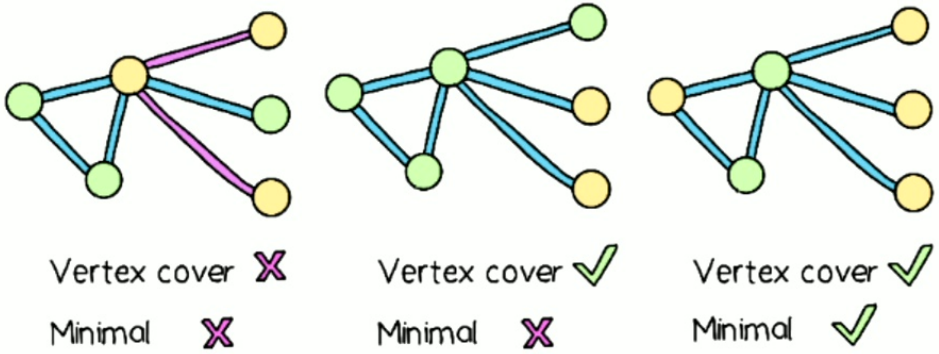
Let’s try this in PennyLane!

What is combinatorial optimization?

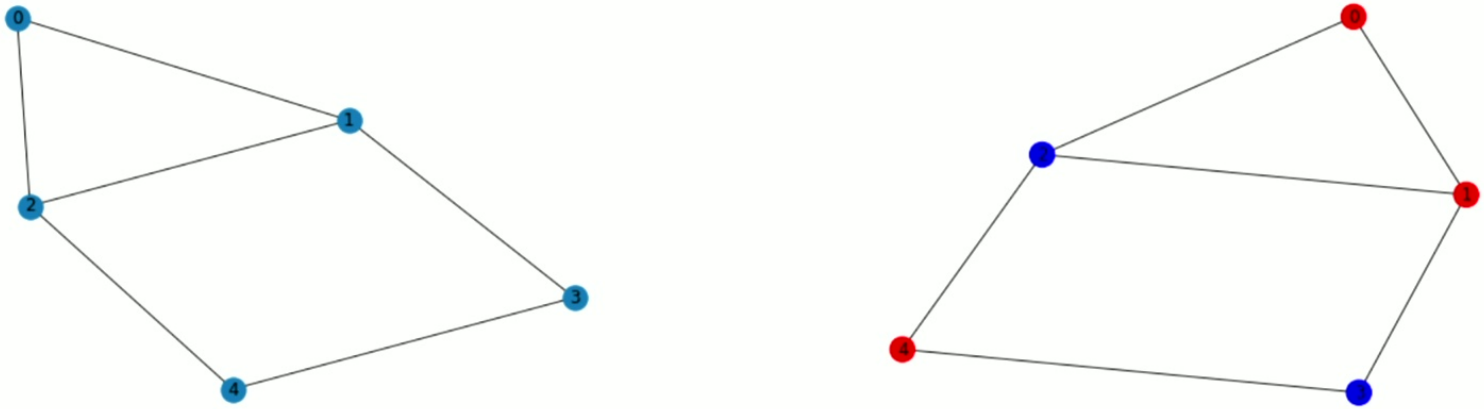


Another Potential Application of Optimization with Quantum Circuits

Finding an optimal combination among the set of all possible combinations. Examples:

Knapsack problem, Minimum vertex cover, MaxCut

The MAXCUT problem



Partition a graph into two sets of vertices

If we maximize the number of edges between elements of different colours (sets of vertices), then we have a MAXCUT of the graph. Finding this partition is a combinatorial optimization problem.

Mathematical formulation of MAXCUT

Maximize the function:

$$C(\vec{s}) = \frac{1}{2} \sum_{(i,j)\in E} (1 - s_i s_j)$$

Where the s take the value 1 if s is in partition 1, and the value -1 if it's in partition 2.

Quantum Formulation

Map cost function into Cost Hamiltonian

$$\hat{C} = -\frac{1}{2} \sum_{(i,j) \in E} (\mathbb{1} - Z_i Z_j)$$

Amounts to finding the ground state of this cost Hamiltonian. Let's implement this Hamiltonian in PennyLane for our MAXCUT graph.

QAOA Theory

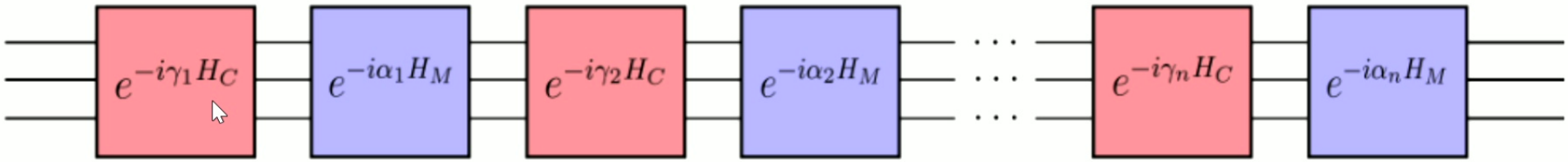
Based on **Adiabatic theorem.** If we evolve the ground state of H_0 under the time dependent Hamiltonian

$$H(t) = (1-t)H_0 + tH_1, \quad t \in [0,1],$$

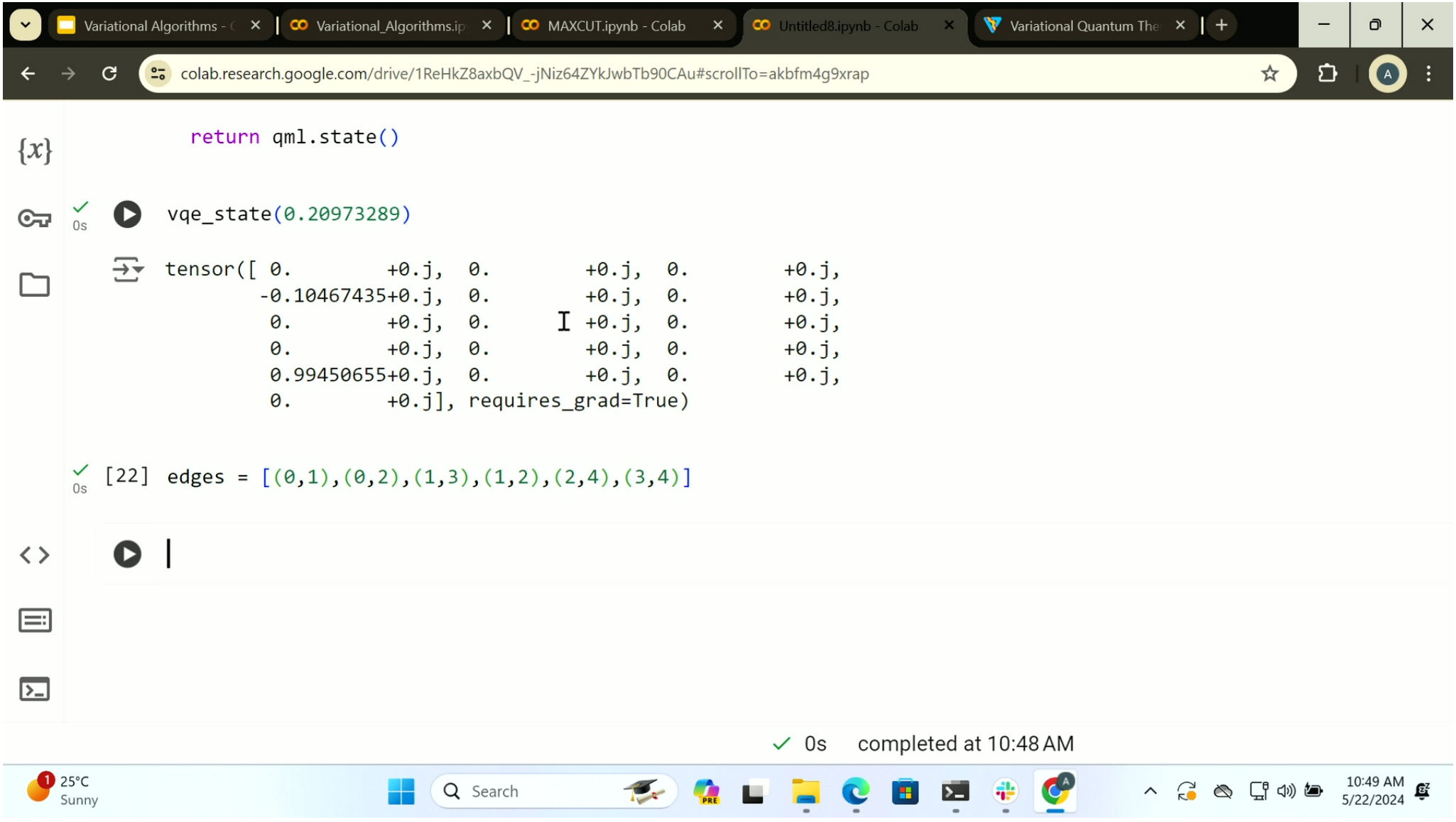
We end up in the ground state of H_1.

Strategy: Start in the ground state of a Hamiltonian we know (mixer Hamiltonian), and evolve adiabatically to end up in ground state of target Hamiltonian.

Implementation



Circuit above implements an **approximate** adiabatic evolution between the mixer and target Hamiltonian, also knowns as **cost Hamiltonian.**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return qml.state()
vqe_state(0.20973289)
tensor([0. +0.j, 0. +0.j, 0. +0.j,
-0.10467435+0.j, 0. +0.j, 0. +0.j,
0. +0.j, 0. +0.j, 0. +0.j,
0. +0.j, 0. +0.j, 0. +0.j,
0.99450655+0.j, 0. +0.j, 0. +0.j,
0. +0.j], requires_grad=True)
[22] edges = [(0,1),(0,2),(1,3),(1,2),(2,4),(3,4)]
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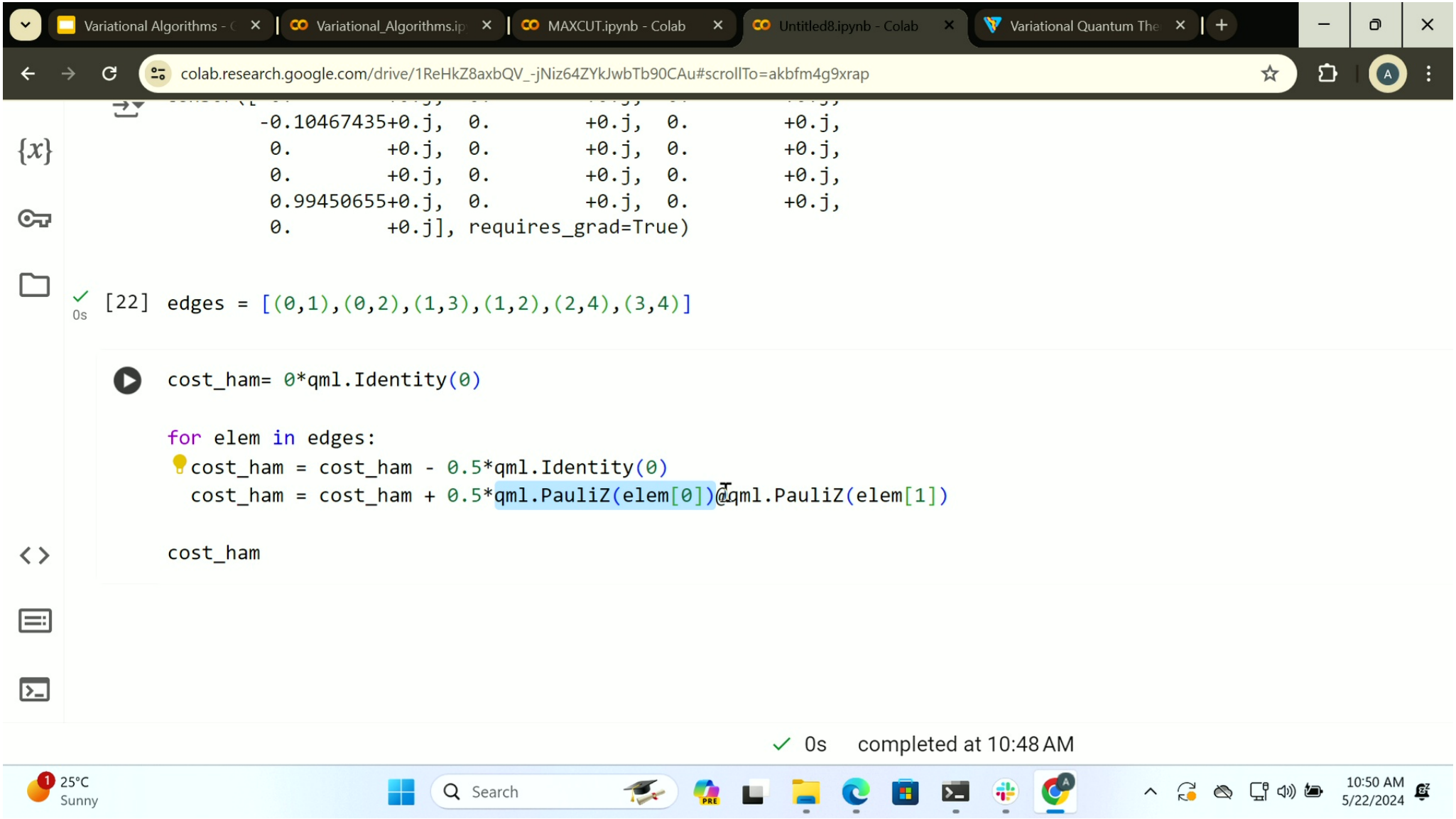
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0. +0.j, 0. +0.j, 0. +0.j,
0. +0.j, 0. +0.j, 0. +0.j,
0.99450655+0.j, 0. +0.j, 0. +0.j,
0. +0.j], requires_grad=True)
[22] edges = [(0,1),(0,2),(1,3),(1,2),(2,4),(3,4)]
0s
cost_ham= 0*qml.Identity(0)
for elem in edges:
cost_ham = cost_ham - 0.5*qml.Identity(0)
cost_ham = cost_ham + 0.5*qml.PauliZ(elem[0])@qml.PauliZ(elem[1])
cost_ham
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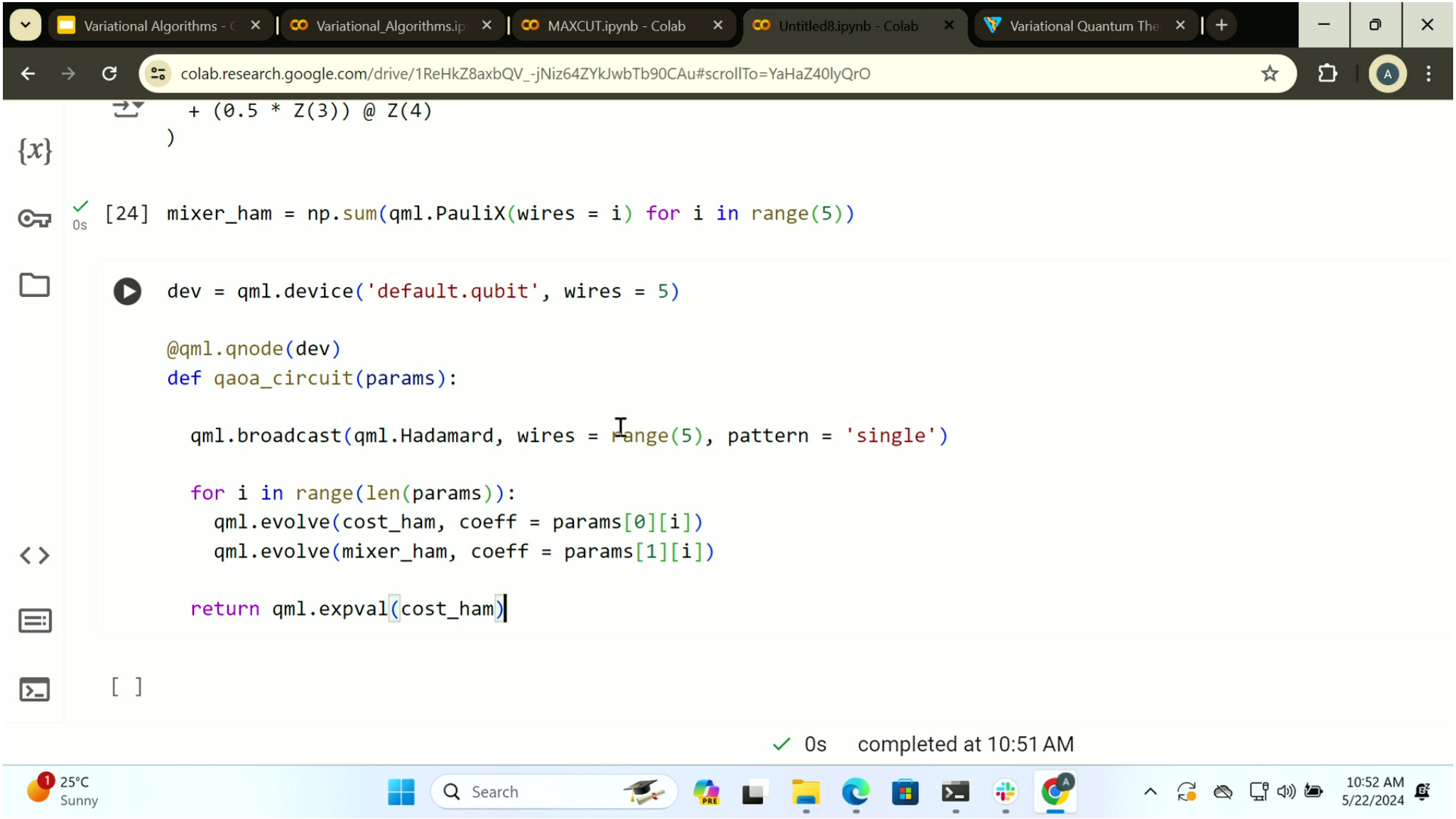
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+ (0.5 * Z(3)) @ Z(4)
)
[24] mixer_ham = np.sum(qml.PauliX(wires = i) for i in range(5))
0s
dev = qml.device('default.qubit', wires = 5)
@qml.qnode(dev)
def qaoa_circuit(params):
qml.broadcast(qml.Hadamard, wires = range(5), pattern = 'single')
for i in range(len(params)):
qml.evolve(cost_ham, coeff = params[0][i])
qml.evolve(mixer_ham, coeff = params[1][i])
return qml.expval(cost_ham)
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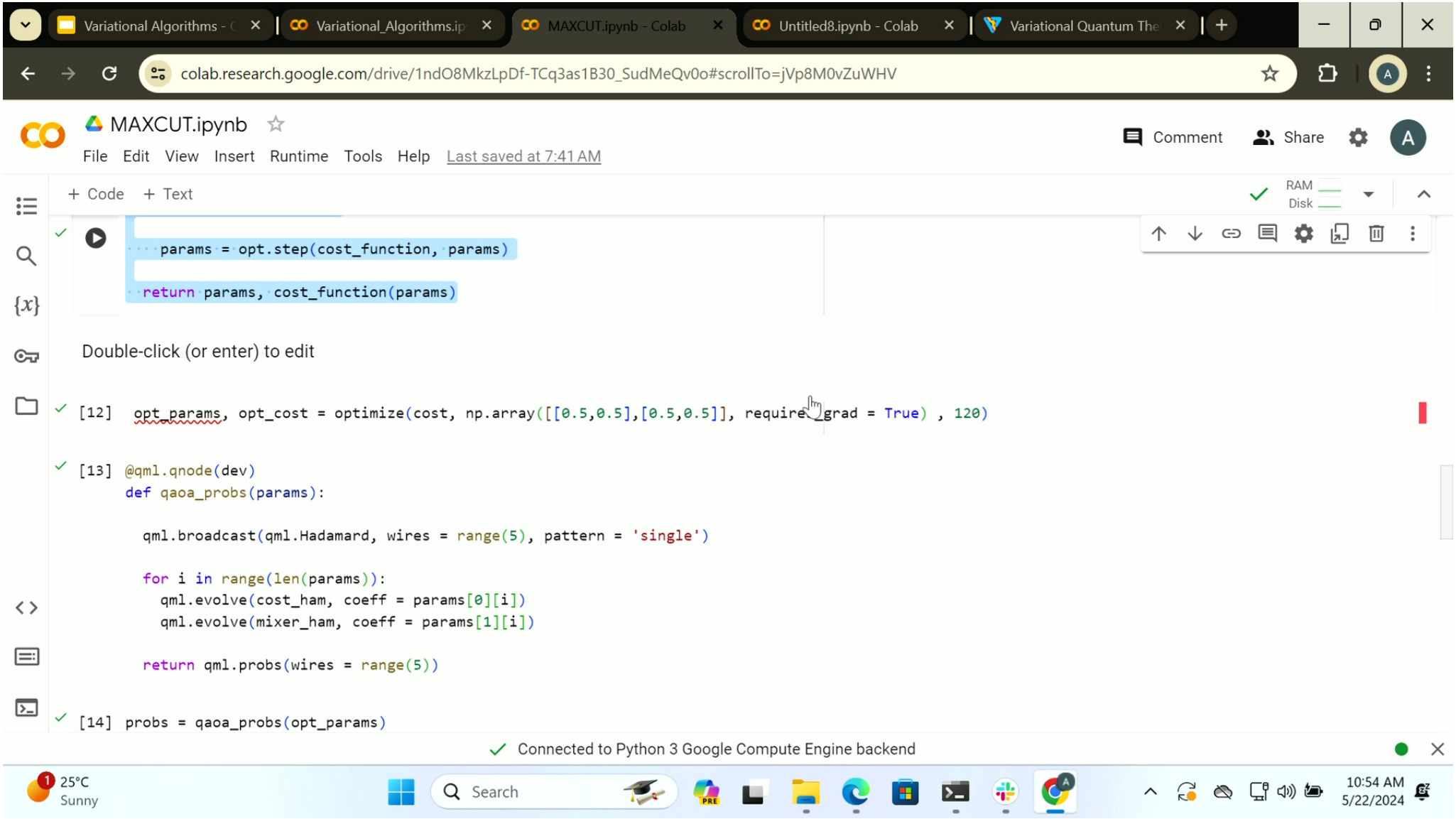
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params = opt.step(cost_function, params)
return params, cost_function(params)
Double-click (or enter) to edit
[12] opt_params, opt_cost = optimize(cost, np.array([[0.5,0.5],[0.5,0.5]], requires_grad = True) , 120)
[13] @qml.qnode(dev)
def qaoa_probs(params):
qml.broadcast(qml.Hadamard, wires = range(5), pattern = 'single')
for i in range(len(params)):
qml.evolve(cost_ham, coeff = params[0][i])
qml.evolve(mixer_ham, coeff = params[1][i])
return qml.probs(wires = range(5))
[14] probs = qaoa_probs(opt_params)
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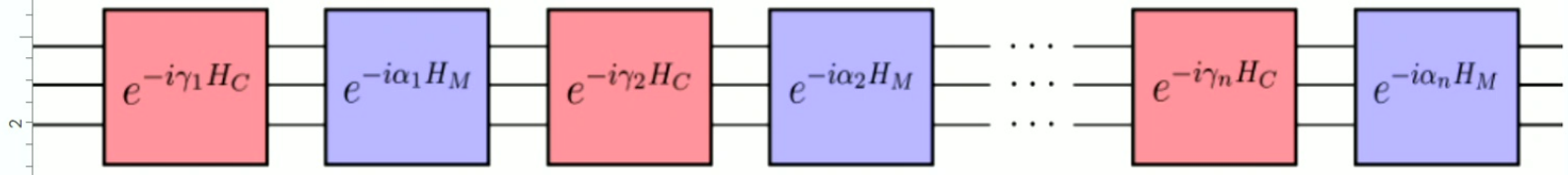
20 Quantum Formulation

21 QAOA Theory

22 Implementation

23 Let's try this in PennyLane!



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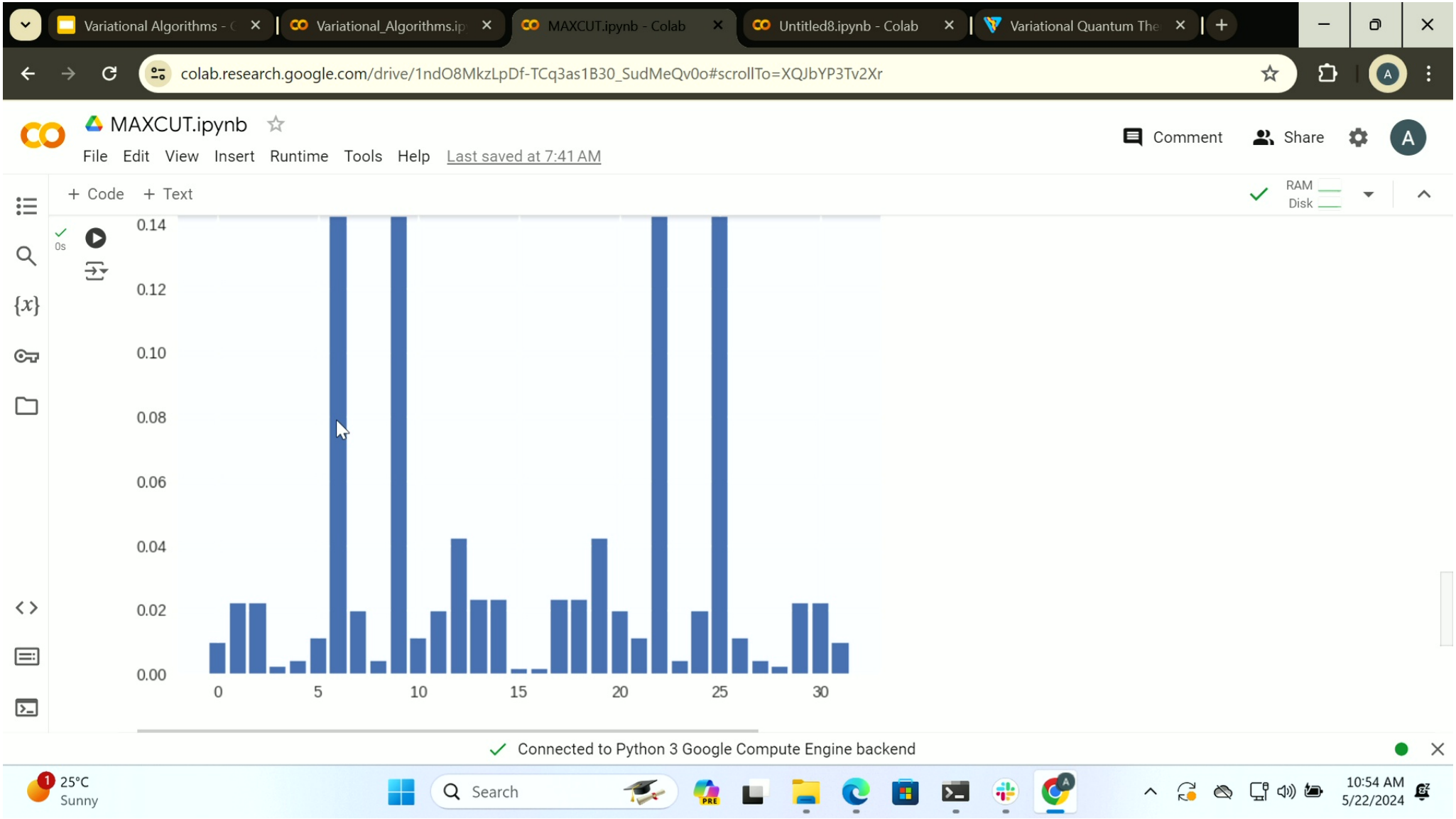
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```
    return qml.probs(wires = range(5))
```

```
[14] probs = qaoa_probs(opt_params)
```

```
from matplotlib import pyplot as plt
plt.style.use("seaborn")
plt.bar(range(2 ** 5), probs)
plt.show()
```

```
<ipython-input-15-6f6f4133b234>:2: MatplotlibDeprecationWarning: The seaborn styles shipped by Matplotlib are deprecated since 3.6, as they no longer
  plt.style.use("seaborn")
```

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