CPEN 400Q / EECE 571Q Lecture 17
Noisy device simulation, VQE, and error mitigation

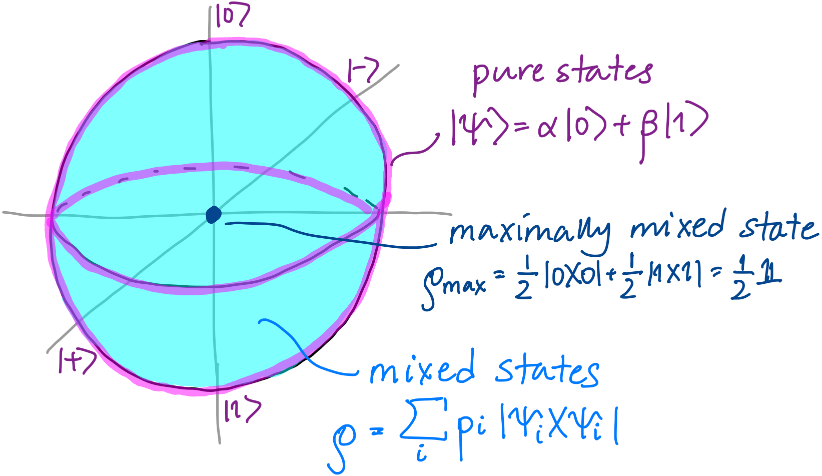
Tuesday 15 March 2022

Announcements

- Assignment 4 coming this week (will be due at end of term)
- Second-last quiz today
- New version of PennyLane out today, v0.22 (we will not be updating, but check it out: `https://pennylane.ai/blog/2022/03/pennylane-v022-released/`)

Last time

We introduced *density matrices* and *mixed states*.



Last time

We saw how states, operations, and measurements look like on mixed vs. pure states.

	Pure state	Pure state ρ	Mixed state ρ
States	$\lvert\psi\rangle = \alpha\lvert 0\rangle + \beta\lvert 1\rangle$	$\rho = \lvert\psi\rangle\langle\psi\rvert$	$\rho = \sum_i p_i \lvert\psi_i\rangle\langle\psi_i\rvert$
Ops.	$\lvert\psi'\rangle = U\lvert\psi\rangle$	$\rho' = U\rho U^\dagger$ $\lvert\psi'\rangle\langle\psi'\rvert = U\lvert\psi\rangle\langle\psi\rvert U^\dagger$	$\rho' = U\rho U^\dagger$
Meas.*	$\lvert\langle\varphi_i\lvert\psi\rangle\rvert^2$ $\langle\psi\rvert B\lvert\psi\rangle$	$\mathrm{Tr}(\lvert\varphi_i\rangle\langle\varphi_i\rvert \cdot \lvert\psi\rangle\langle\psi\rvert)$ $\mathrm{Tr}(B\rho)$	$\mathrm{Tr}(P_i\rho)$ $\mathrm{Tr}(B\rho)$

* where $\{\varphi_i\}$ form an orthonormal basis, and $\{P_i\}$ may be the associated set of projectors $P_i = \lvert\varphi_i\rangle\langle\varphi_i\rvert$ or more generally a POVM (in either case, $\sum_i P_i = I$).

Learning outcomes

- Add simple noise to quantum circuits in PennyLane
- Perform simulations on noisy devices using PennyLane plugins
- Mitigate noise using zero-noise extrapolation

Quantum channels and noise

Noise occurring in quantum systems is represented by **quantum channels**.

A quantum channel Φ *maps* states to other states.

$$\rho \to \rho' = \Phi(\rho)$$

More formally, quantum channels are linear CPTP (Completely Positive, Trace-Preserving) maps.

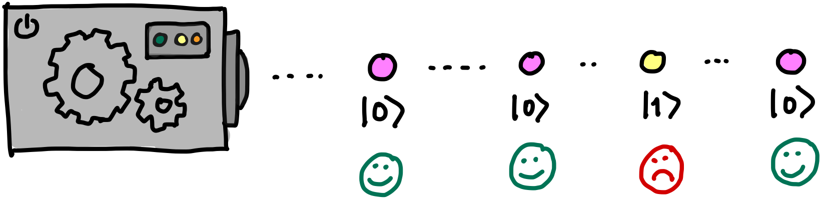
Example: applying a unitary U is a channel, $\mathcal{U}$.

$$\rho \to \rho' = \mathcal{U}(\rho) = U \rho U^\dagger$$

The bit flip channel

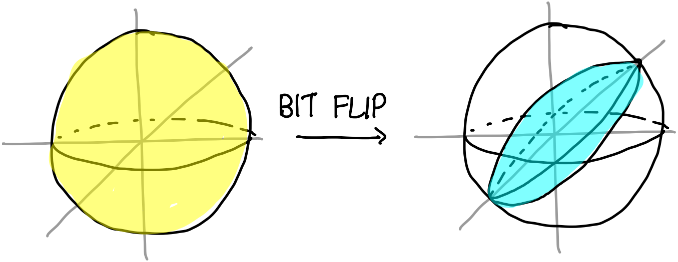
Suppose a “bit flip” (Pauli X) error occurs with probability p.

$$\mathcal{E}(\rho) = (1-p)\cdot\rho + p\cdot X\rho X$$



The bit flip channel

We can visualize the effects of such a channel by observing how it deforms the Bloch sphere.



x : same
yz : contracts (factor 1-2p)

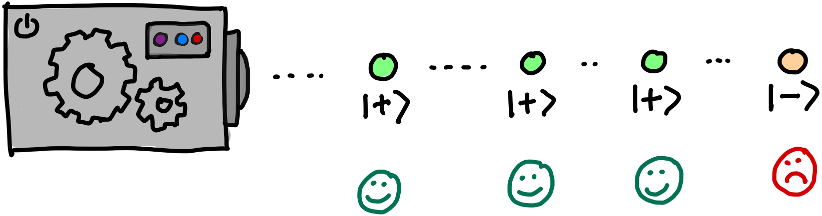
$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

bit flip: $\frac{1}{\sqrt{2}}(|1\rangle + |0\rangle)$

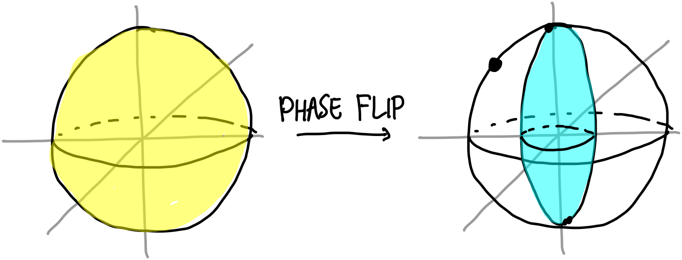
The phase flip channel

Suppose a "phase flip" (Pauli Z) error occurs with probability p.

$$\mathcal{E}(\rho) = (1-p)\cdot\rho + p\cdot Z\rho Z$$



The phase flip channel



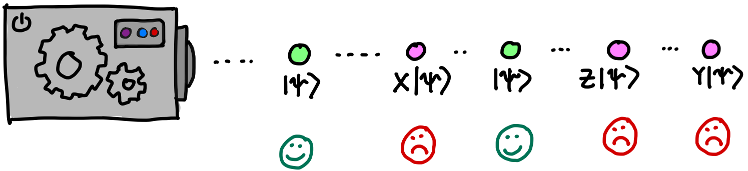
z: same
xy: contracts
(factor $1-2p$)

$$|\psi\rangle\langle\psi| \rightarrow (1-p)|\psi\rangle\langle\psi| + pZ|\psi\rangle\langle\psi|Z$$

The depolarizing channel

Suppose each Pauli error occurs with probability $p/3$. This is called the *depolarizing channel*.

$$\mathcal{E}(\rho) = (1-p)\cdot\rho + \frac{p}{3}\cdot X\rho X + \frac{p}{3} Y\rho Y + \frac{p}{3} Z\rho Z$$



$$X\rho X^\dagger \rightarrow X^\dagger = X$$

The depolarizing channel

$$\mathcal{E}(\rho) = (1-p)\rho + \frac{p}{3}X\rho X + \frac{p}{3}Y\rho Y + \frac{p}{3}Z\rho Z^\dagger$$

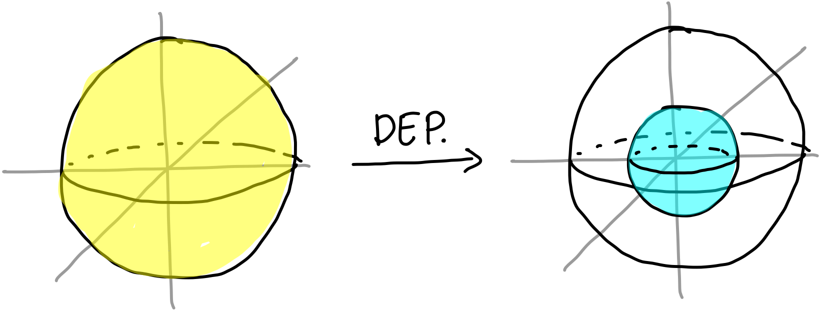
can also be written as

$$\mathcal{E}(\rho) = (1-p)\rho + p\frac{\mathbb{1}}{2}$$

Think of this as outputting ρ w/probability $1-p$, and maximally mixed state with probability p.

$$\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{2}\mathbb{1}$$

The depolarizing channel



... let's add some noise to quantum circuits.

Comparing density matrices

How can we quantify “how much” error occurs? How close is $\sigma = \mathcal{E}(\rho)$ to ρ?

One common way is the **trace distance**:

$$\mathrm{Tr}(\rho, \sigma) = \frac{1}{2}\|\rho - \sigma\|_1 = \frac{1}{2}\mathrm{Tr}\left(\sqrt{(\rho-\sigma)^\dagger(\rho-\sigma)}\right)$$

Value of trace distance is bounded by $0 \leq T(\rho, \sigma) \leq 1$. *Lower* trace distance is better.

Comparing density matrices

Another is the **fidelity**:

$$F(\rho,\sigma) = \left(\mathrm{Tr}\sqrt{\sqrt{\rho}\,\sigma\sqrt{\rho}}\right)^2$$

Value is bounded by $0 \leq F(\rho,\sigma) \leq 1$. *Higher* fidelity is better.

Can show that if $\rho = |\psi\rangle\langle\psi|$ is pure, then

$$F(\rho,\sigma) = \langle\psi|\sigma|\psi\rangle$$

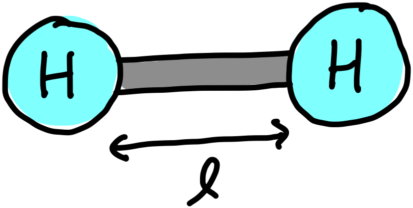
If $\sigma = |\varphi\rangle\langle\varphi|$ is also pure,

$$F(\rho,\sigma) = |\langle\varphi|\psi\rangle|^2$$

VQE on (simulated) noisy hardware

VQE on a noisy device

Let's solve a (small) *quantum chemistry* problem: find the ground state energy of H_2.



H_2 is a molecule with 2 electrons.

$|0\,1\,1\,0\rangle$ orbital

The Hamiltonian for H_2 can be written using 4 qubits.

Qubits correspond to molecular orbitals that are either *occupied* ($|1\rangle$) or *unoccupied* ($|0\rangle$).

The ground state has the form:

$$|\psi_g\rangle = \cos\frac{\theta}{2}|1100\rangle - \sin\frac{\theta}{2}|0011\rangle$$

What gates should we use to prepare this state?

$|0101\rangle \rightarrow |0111\rangle$

$|0110\rangle \rightarrow |1100\rangle$

$|0011\rangle$

A **single excitation** has the form

$$G(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta/2) & -\sin(\theta/2) & 0 \\ 0 & \sin(\theta/2) & \cos(\theta/2) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

This has the action

$$G|01\rangle = \cos\frac{\theta}{2}|01\rangle + \sin\frac{\theta}{2}|10\rangle$$
$$G|10\rangle = \cos\frac{\theta}{2}|10\rangle - \sin\frac{\theta}{2}|01\rangle$$

$$G|01\rangle = \cos(\theta/2)|01\rangle + \sin(\theta/2)|10\rangle$$
$$G|10\rangle = \cos(\theta/2)|10\rangle - \sin(\theta/2)|01\rangle$$

(In PennyLane: `qml.SingleExcitation`).

Single excitations can be visualized like so:

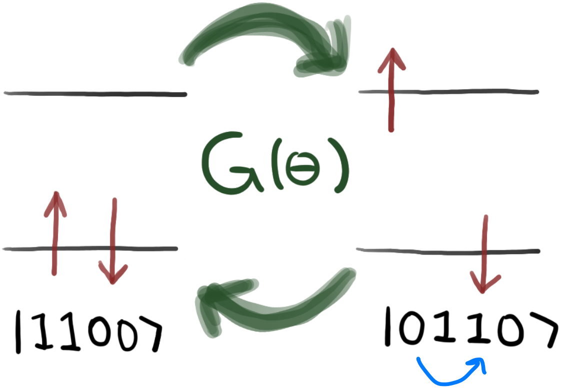
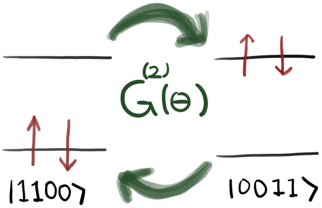


Image credit: Givens rotation demo, https://pennylane.ai/qml/demos/tutorial_givens_rotations.html

Similarly, there are double excitations:



This has the action

$$G^{(2)}|0011\rangle = \cos\frac{\theta}{2}|0011\rangle + \sin\frac{\theta}{2}|1100\rangle$$
$$G^{(2)}|1100\rangle = \cos\frac{\theta}{2}|1100\rangle - \sin\frac{\theta}{2}|0011\rangle$$

(In PennyLane: `qml.DoubleExcitation`).

Image credit: Givens rotation demo, https://pennylane.ai/qml/demos/tutorial_givens_rotations.html

VQE on a noisy device

So to produce

$$|\psi_g\rangle = \cos(\theta/2)|1100\rangle - \sin(\theta/2)|0011\rangle$$

we will

1. prepare the state $|1100\rangle$
2. apply a double excitation

Then we run VQE to find the optimal θ.

We will run this on an ideal device, and a device with a simulated noise model based on a real processor using PennyLane-Qiskit.

Clearly noise is a problem. How do we measure the quality of noisy quantum devices?

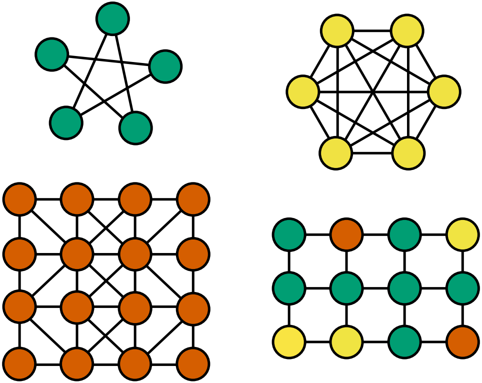


Image credit: quantum volume demo, `https://pennylane.ai/qml/demos/quantum_volume.html`

Comparing quantum computers

It is challenging to characterize, benchmark, and to compare quantum computers: it's more than just number of qubits.

- error rates
- qubit connectivity
- software/compiler quality
- gate operation times
- size of problem it can solve
- size of meaningful problem it can solve
- ...

Comparing supercomputers

It's more than just number of cores: comparison based on LINPACK benchmark (FLOPS while solving dense linear system).

https://www.top500.org/lists/top500/2021/11/

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442,010.0	537,212.0	29,899
2	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	200,794.9	10,096
3	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438

Comparing quantum computers

Many competing metrics proposed by competing companies:

- quantum volume (IBM)
- CLOPS: circuit layer operations per second (IBM)
- algorithmic qubits (IonQ)
- Q-score (Atos)

(I will post a note on Piazza with links to some articles / tutorials)

All this goes to say: current quantum hardware is noisy. Noise comes from a variety of sources, and depends on the qubit technology and architecture.

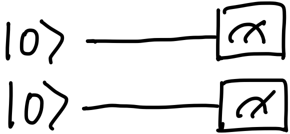
We need to do a combination of:

- Better-characterizing the behaviour of devices to learn how to improve their operation
- Processing the results to mitigate the effects of noise as much as possible

Today we will consider the latter.
(We will do the former another day, time permitting.)

☆ We stopped here.

Errors can occur in the measurement process where states are read out incorrectly.

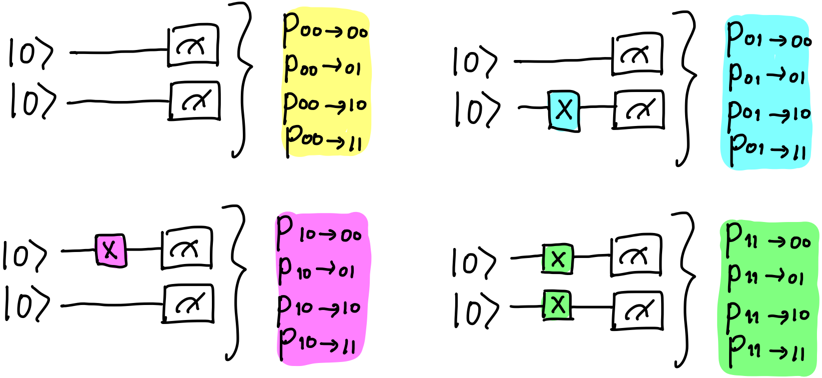


00 :	0.95	$p_{00\to 00}$
01 :	0.02	$p_{00\to 01}$
10 :	0.02	$p_{00\to 10}$
11 :	0.01	$p_{00\to 11}$

These kinds of errors are quite straightforward to mitigate.

Measurement error mitigation

Check what happens with all possible input states:



Measurement error mitigation

We can put the results from our calibration circuits into a matrix:

$$M = \begin{bmatrix} p_{00\to 00} & p_{01\to 00} & p_{10\to 00} & p_{11\to 00} \\ p_{00\to 01} & p_{01\to 01} & p_{10\to 01} & p_{11\to 01} \\ p_{00\to 10} & p_{01\to 10} & p_{10\to 10} & p_{11\to 10} \\ p_{00\to 11} & p_{01\to 11} & p_{10\to 11} & p_{11\to 11} \end{bmatrix}$$

Can suppose that the probability vector P_{noisy} we get at the end of a quantum algorithm is related to the ideal one, P_{ideal}, under multiplication by M since that's what we see:

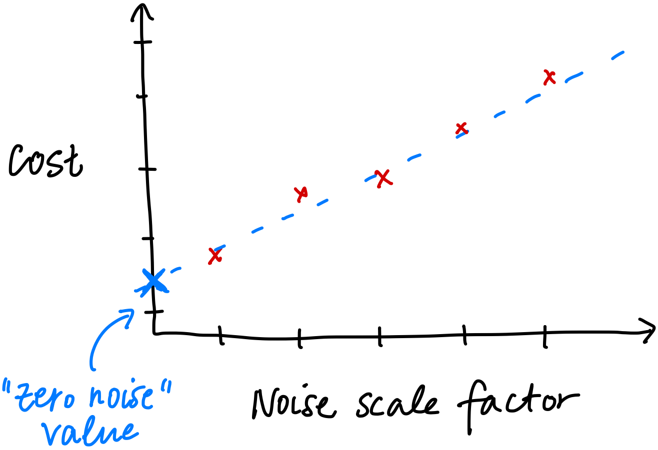
$$P_{noisy} = MP_{ideal}$$

So to get the ideal results:

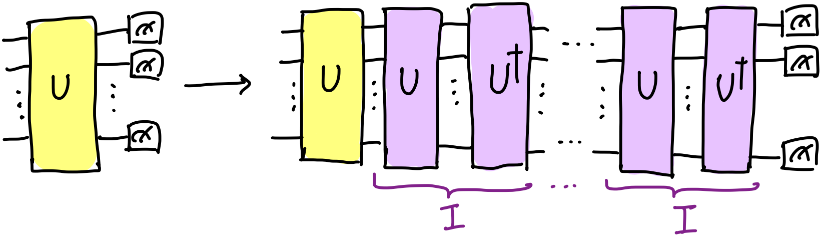
$$P_{ideal} = M^{-1}P_{noisy}$$

Gate error mitigation: zero-noise extrapolation

Modify the circuits to systematically *increase* scale of the noise, then extrapolate down to the zero-noise limit.



Unitary folding



Let's code up a very basic version of this in PennyLane.

More sophisticated version: Python package `mitiq`
`https://github.com/unitaryfund/mitiq`

Next time

Content:

- Quantum approximate optimization algorithm

★ error mitigation

Action items:

1. Final project

Recommended reading:

- Nielsen and Chuang Ch. 8
- Qiskit tutorial on measurement error mitigation: `https://qiskit.org/textbook/ch-quantum-hardware/measurement-error-mitigation.html`
- `mitiq` documentation, for more fun error mitigation: `https://mitiq.readthedocs.io/en/stable/guide/guide.html`