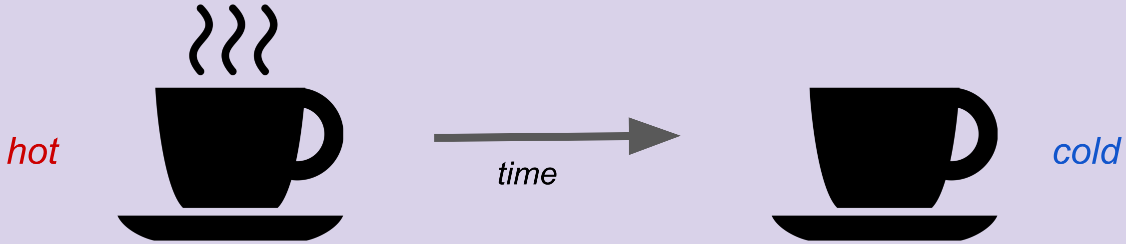
Exploring Localization and Excited States with VQE

Eli Chertkov, Ryan Levy, James Allen, Abid Khan, and Di Luo
University of Illinois at Urbana-Champaign
(graduate students from Clark group)

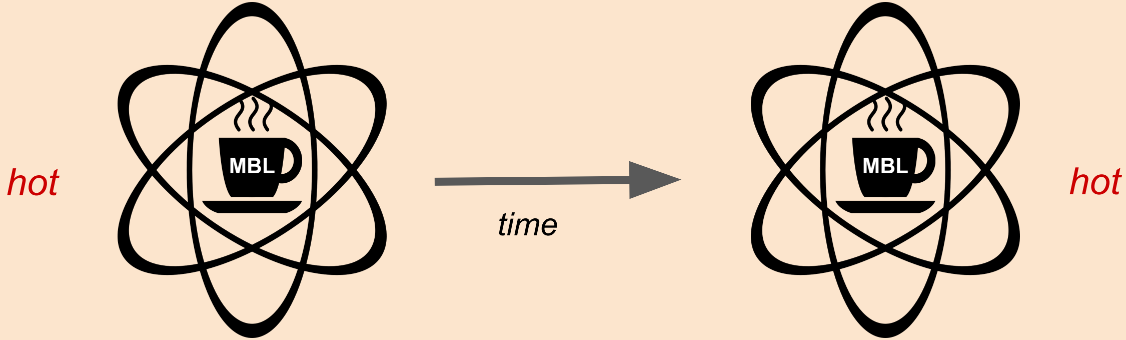
Qiskit Summer Jam 2020
QuarantineQbits project presentation
July 1, 2020

Introduction to many-body localization (MBL)

Classical matter (and most quantum matter) thermally equilibrates over time

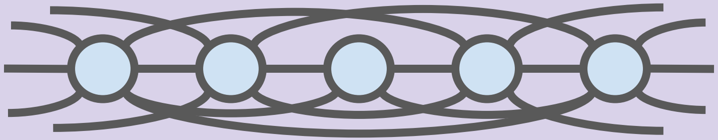
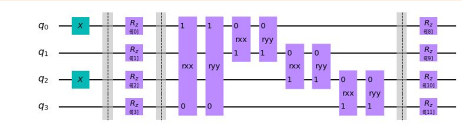
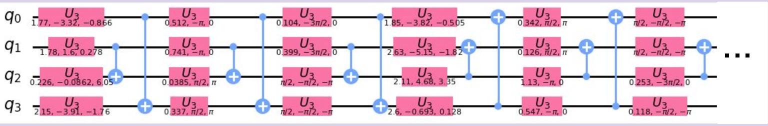


MBL quantum systems do *not* thermally equilibrate, like a never-cooling coffee cup



Excited states in MBL vs usual (ergodic) quantum systems

A key property of MBL systems is that their excited states have *low entanglement*.

	MBL	**Ergodic**
Entanglement (Excited States)	 *area-law* (constant in 1D)	 *volume-law* (linear in system size in 1D)
Circuit Representation (1D)	 constant-depth quantum circuit	 deep quantum circuit

Low-depth variational circuit states can accurately represent MBL excited states!

Project goals

Our goal was to observe **many-body localization** (MBL) on a quantum computer. To reach this goal:

We implemented two quantum algorithms in Qiskit

Variance variational quantum eigensolver (**VVQE**)

$\hat{H}$ → **VVQE** → $|\psi(\theta^*)\rangle$

Hamiltonian *Approximate excited state*

A modified version of VQE that we developed to find excited states instead of ground states.

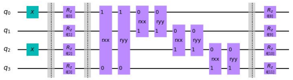
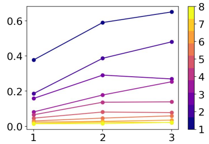
The Bell-Basis algorithm (**BBA**)

$|\psi\rangle$ → **BBA** → S_2

Quantum state *(Renyi) entanglement entropy*

An algorithm for calculating the entanglement entropy of a quantum state.

We ran these algorithms with Qiskit simulators and observed signatures of an MBL transition

$\hat{H}$  → **VVQE** → $|\psi(\theta^*)\rangle$  → **BBA** → 

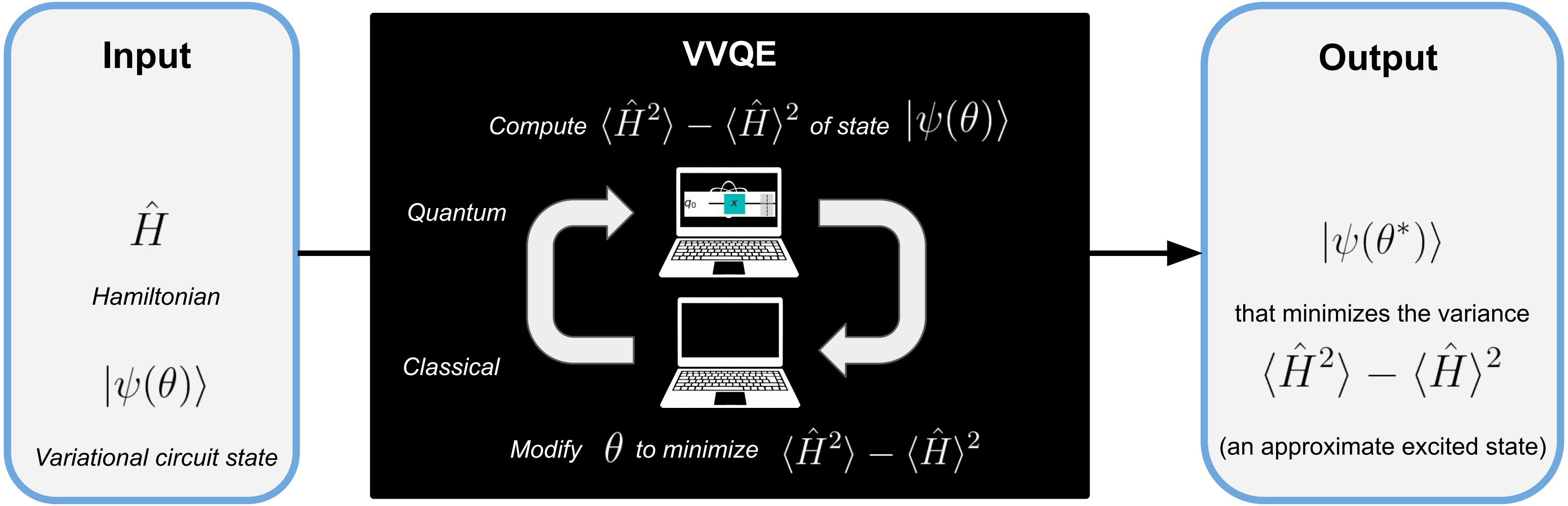
MBL Hamiltonian

Approximate MBL excited state

Entanglement of MBL excited state

Variance variational quantum eigensolver (VVQE)

VVQE minimizes the energy variance of a variational quantum circuit. The variance is computed on a quantum computer, while the optimization is performed on a classical computer.



Our implementation of VVQE is based on the VQE class built in Qiskit Aqua.

Peruzzo et al. Nature Communications 5, 4213 (2014).

See Higgott et. al. Quantum 3, 156, (2019) for an alternative VQE-based method for finding excited states.

Bell-Basis algorithm (BBA)

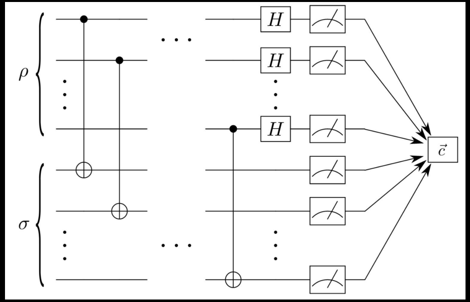
BBA is a quantum algorithm for measuring overlaps and entanglement entropies of quantum states. In Qiskit, we implement a variant from [*Cincio et al. New J. Phys (2018).*](#)

Input

$$\rho, \sigma$$

States (density matrices) prepared by quantum circuits

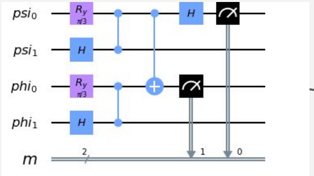
BBA Circuit



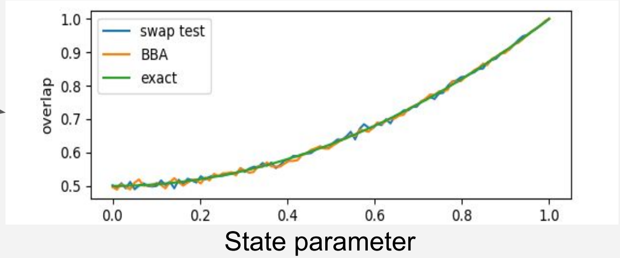
Output

$$\mathrm{tr}(\rho\sigma)$$

Overlap of the states



A 2 qubit test of BBA versus an alternative algorithm (SWAP test)



This overlap directly measures the second Renyi entanglement entropy

$$S_2 = -\log(\mathrm{tr}(\rho^2))$$

when $\rho = \sigma$

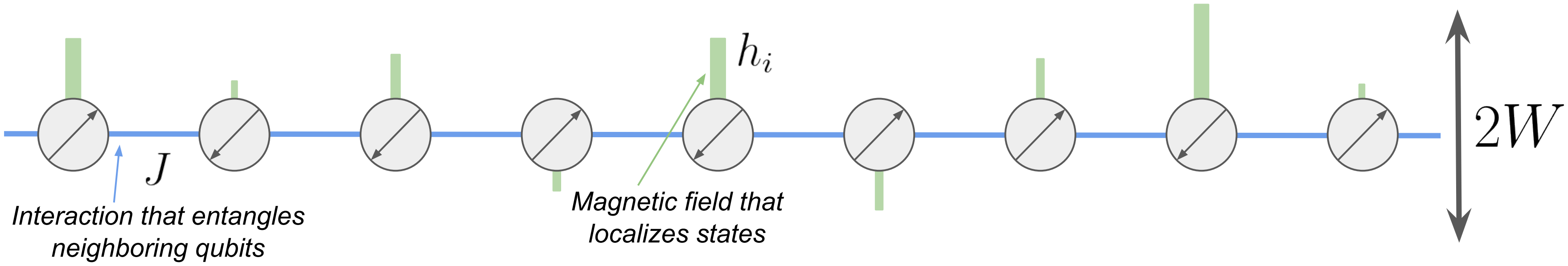
The Hamiltonian we studied

We examined the "standard model of MBL," the disordered 1D Heisenberg model:

$$\hat{H} = \frac{1}{4}\sum_{i=1}^{N-1} J\left(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \sigma_i^z\sigma_{i+1}^z\right) + \frac{1}{2}\sum_{i=1}^{N} h_i\sigma_i^z$$

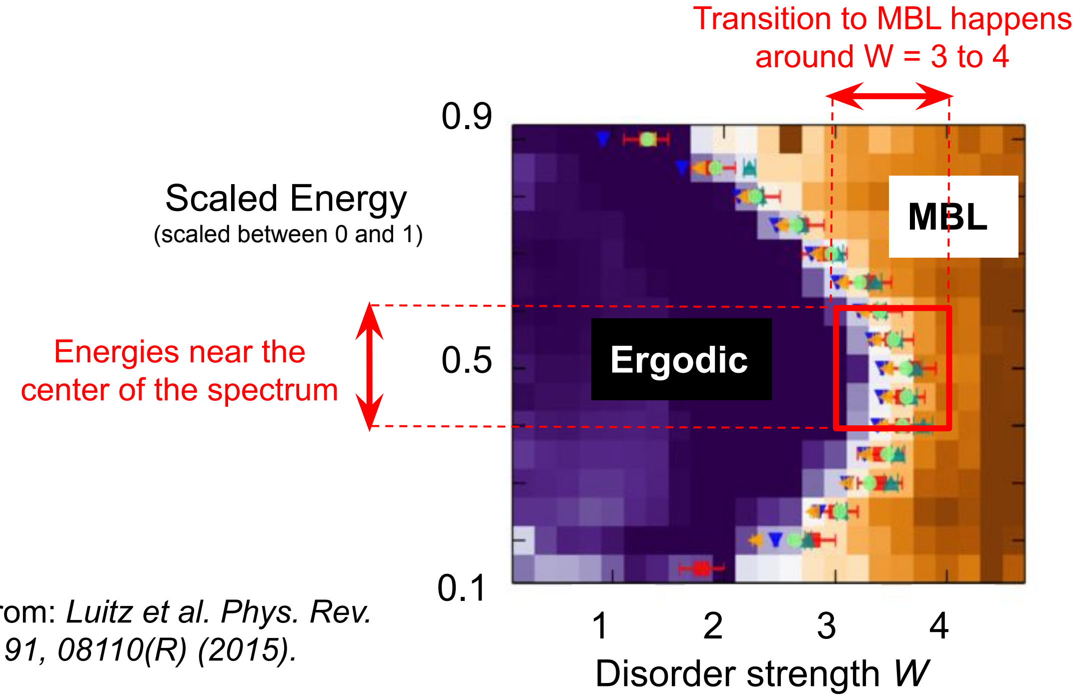
where σ_i^α are Pauli matrices and h_i are random magnetic fields drawn from a uniform distribution between $[-W, W]$ and W is the **disorder strength**.

This is a model for a disordered chain of interacting spins (or qubits):



Past numerical results on this Hamiltonian

From exact diagonalization calculations on the 1D Heisenberg model, researchers have observed an ergodic to MBL transition by looking at excited states.



From: *Luitz et al. Phys. Rev. B 91, 08110(R) (2015).*

Following these observations, we want to find excited states near the center of the spectrum (where the unscaled energy is near zero) and expect a transition at W = 3 to 4.

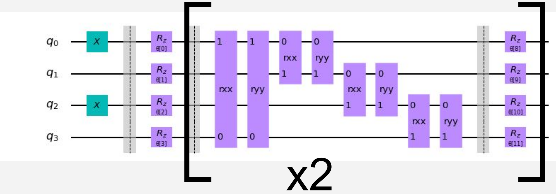
Details of our Qiskit calculations

Variational form

ExcitationPreserving
(chosen because it obeys Sz symmetry)

4 qubit example

$$|\psi(\theta)\rangle \quad = $$



(reps=2, entanglement='sca')

VVQE Optimizer

SLSQP (maxiter = 500)

Simulators

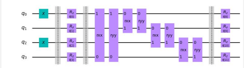
statevector_simulator for VVQE
(due to limited time)
qasm_simulator for BBA

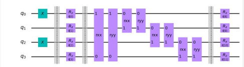
Workflow

1. Generate disordered realizations (samples) of H

2. Run VVQE[1] on each H to get an excited state.

3. Run BBA on each excited state to measure entropy.

$\hat{H}_1$  VVQE → $|\psi(\theta_1^*)\rangle$  BBA → $S_{2,1}$

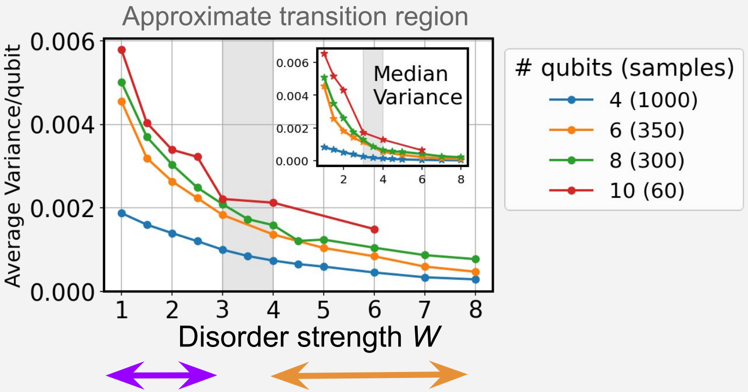
$\hat{H}_2$  VVQE → $|\psi(\theta_2^*)\rangle$  BBA → $S_{2,2}$

... ...

[1]In practice, to target states near the center of the spectrum, we first ran usual VQE on H^2 to get states near zero energy. Then we ran VVQE.

VVQE results

Average Performance

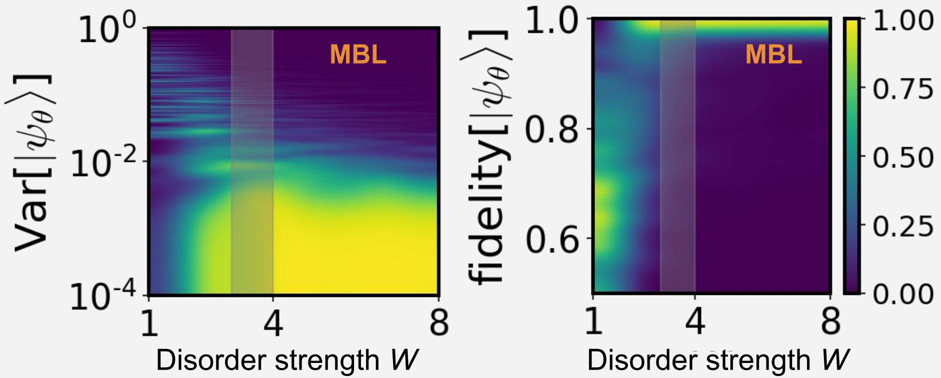


In **ergodic** phase, the variance significantly increases.

We find excellent variance in the **MBL** regime.

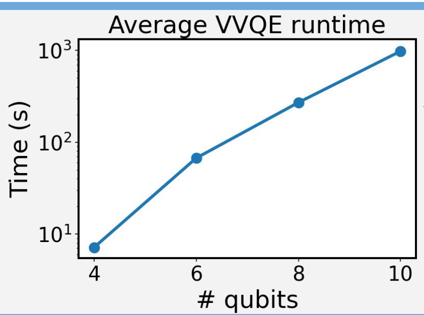
Accuracy at 8 qubits

(Interpolated histograms with maxima at 1)



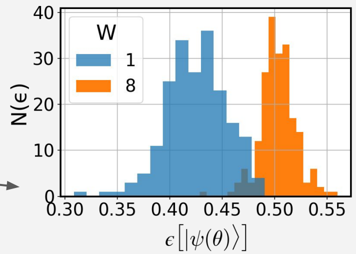
These histograms show that in the **MBL** phase, our variational circuits have high overlap (fidelity) with the true excited states and low variance, but in the **ergodic** phase have low overlap and bad variance.

Profiling



Timing of VVQE with `statevector_simulator`.

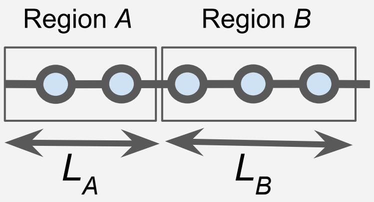
Distribution of energies of VVQE output states. We successfully found states near center of the spectrum, though they were shifted for low disorder.



Scaled energy (0 to 1)

BBA results

Using BBA, we compute entanglement between two subsystems of different sizes.



In **ergodic** phase, we expect volume-law scaling:

$$S_2 \propto L_A \quad (dS_2/dL_A = \text{constant})$$

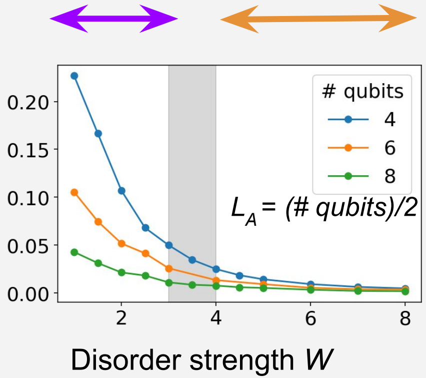
In **MBL** phase, we expect area-law scaling:

$$S_2 \propto \text{constant} \quad (dS_2/dL_A = 0)$$

Entropy (Half cut) vs Disorder

In **ergodic** phase, our variational ansatz gets worse with increasing number of qubits,

$\langle S_2 \rangle$/(# qubits)



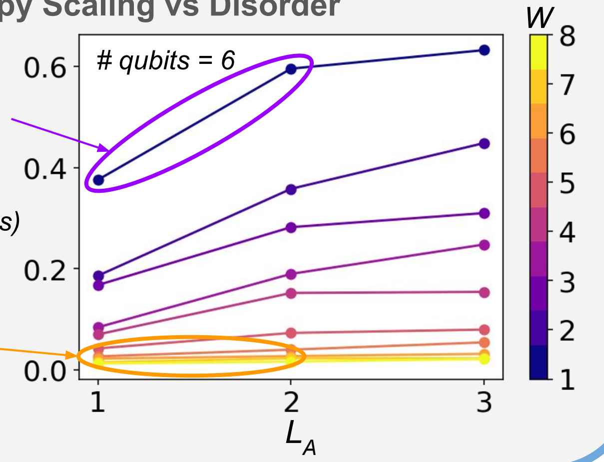
In **MBL** regime, our ansatz does well for all system sizes.

Entropy Scaling vs Disorder

In **ergodic** phase, entropy slope is non-zero.

$\langle S_2 \rangle$/(# qubits)

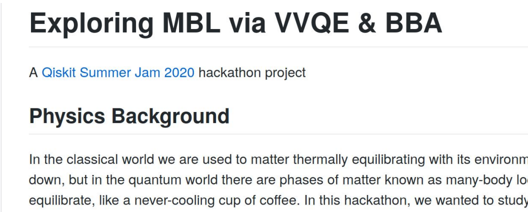
In **MBL** phase, entropy slope is nearly zero.



Summary and conclusions

- **Goal:** Simulate MBL on a noisy near-term quantum computer.
- **We implemented two quantum algorithms in qiskit:**
  - Our new quantum algorithm, the variance variational quantum eigensolver (**VVQE**)
  - The Bell-Basis algorithm (**BBA**)
- **We used the algorithms to measure the entanglement of excited states:**
  - We used our VVQE algorithm to find random excited states of the “standard model of MBL.”
  - We used BBA to measure the entanglement entropy of the excited states.
  - We found signatures of an MBL transition both in the performance of the VVQE algorithm and in the entropies measured by BBA.
- **Future outlook:**
  - The quantum community can use VVQE to study excited states in other contexts.
  - IBM’s noisy quantum devices could directly probe MBL transitions using our methods.
- **Our code:**
  - Our github (including tutorials of VVQE and BBA and our generated data):

    https://github.com/abid1214/mbl-vvqe-bba



Exploring MBL via VVQE & BBA

A Qiskit Summer Jam 2020 hackathon project

Physics Background

In the classical world we are used to matter thermally equilibrating with its environm
down, but in the quantum world there are phases of matter known as many-body lo
equilibrate, like a never-cooling cup of coffee. In this hackathon, we wanted to study

Thanks to Bryce Fuller and Qiskit slack!