

Exact simulation of a Quantum Phase Transition on a quantum computer

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Motivation

Disentangling a hamiltonian

Entangling hamiltonian H \longrightarrow Non-interacting hamiltonian \tilde{H}
(hard to simulate) (easy to simulate)

$$H = U_{dis} \tilde{H} U_{dis}^\dagger$$

$$\begin{array}{lcl} H|\varphi_i\rangle = \epsilon_i|\varphi_i\rangle & \longrightarrow & HU_{dis}|\psi_i\rangle = \epsilon_i U_{dis}|\psi_i\rangle \\ \tilde{H}|\psi_i\rangle = \epsilon_i|\psi_i\rangle & & H|\varphi_i\rangle = \epsilon_i|\varphi_i\rangle \end{array}$$

$$\tilde{H} = \sum_i \epsilon_i \sigma_i^z \text{ (diagonal hamiltonian):}$$

- Eigenstates $|\psi_i\rangle$ correspond to the computational basis:
 \rightarrow easy to prepare
- Applying unitary operation U_{dis} we obtain H eigenstates $|\varphi_i\rangle$:
 \rightarrow we have access to the whole spectrum
- Simulate time evolution $e^{-itH} = U_{dis} e^{-it\tilde{H}} U_{dis}^\dagger$
- Simulate thermal state $e^{-\beta H} = U_{dis} e^{-\beta\tilde{H}} U_{dis}^\dagger$

Quantum computation

Simulation/computation of quantum mechanics

Richard Feynman, about the exponential growing of complexity of a quantum mechanical system description:

*“The problem is, how can we simulate the quantum mechanics? There are two ways that we can go about it. We can give up on our rule about what the computer was, we can say: **Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws.** Or we can turn the other way and say: **Let the computer still be the same kind that we thought of before—a logical, universal automaton; can we imitate this situation?**”*¹

¹International Journal of Theoretical Physics **21**, Nos. 6/7, 1982.

Quantum computation

Quantum mechanical elements:

- Quantum unit of information: *qubit*
- Quantum logic operation: quantum gates
- Quantum platform for the implementation: ions, superconductors, photons,...

Quantum mechanical rules:

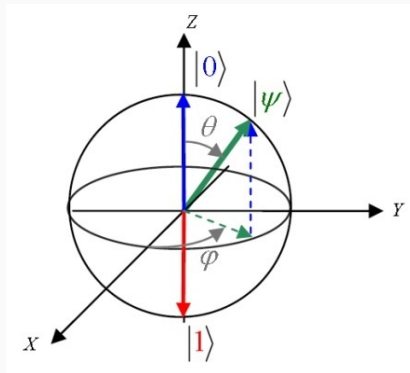
- Unitarity: *reversibility of quantum operations*
- Superposition: *exponential speedup*
- Probabilistic results
- Entanglement: purely quantum property

Qubit

A *qubit* (quantum bit) is a two-state quantum-mechanical system analogue of the classical binary bit.

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\begin{aligned} |\Psi\rangle &= \alpha|0\rangle + \beta|1\rangle \\ &= \cos(\theta/2)|0\rangle + e^{i\varphi} \sin(\theta/2)|1\rangle \end{aligned}$$



Bloch sphere

Qubit

2 qubit state $|a\rangle \otimes |b\rangle \equiv |ab\rangle$:

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Entanglement: $|\psi\rangle_{AB} \neq |\psi\rangle_A \otimes |\psi\rangle_B$. For two qubits, maximal entangled states (Bell basis):

$$|\Phi^\pm\rangle = \frac{1}{\sqrt{2}} (|00\rangle \pm |11\rangle), \quad |\Psi^\pm\rangle = \frac{1}{\sqrt{2}} (|01\rangle \pm |10\rangle)$$

MaxEnt state \rightarrow Max violation of Bell Inequality:

"No physical theory of local hidden variables can ever reproduce all of the predictions of quantum mechanics" (Bell's theorem)

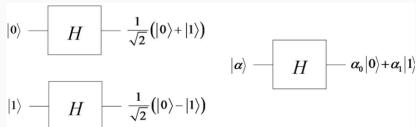
Quantum gates

Quantum gate over n qubits: unitary $2^n \times 2^n$ matrix.

One-qubit gates:

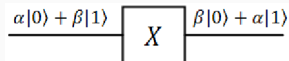
Hadamard: generates superposition

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$



Pauli-X: bit flip, maps $|0\rangle \rightarrow |1\rangle$, $|1\rangle \rightarrow |0\rangle$. Quantum equivalent of classical NOT gate:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$



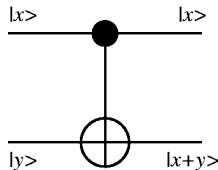
Quantum gates

2-qubit gates:

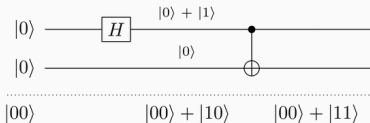
Controlled-X (CNOT): performs the NOT operation on the second qubit if the first qubit is $|1\rangle$, and leaves it unchanged otherwise.

Control qubit	Target qubit	Output	
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$



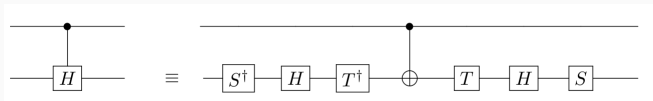
Generates entanglement:



Quantum circuit

Example: Controlled Hadamard gate:

Performs a Hadamard operation if the control qubit is $|1\rangle$:



$$CH = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & 0 & 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}, \quad S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}, \quad T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$$

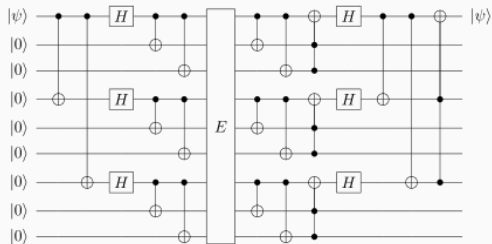
$$\begin{aligned} CH(|01\rangle - |10\rangle)/\sqrt{2} &= (\mathbb{I} \otimes S)(\mathbb{I} \otimes H)(\mathbb{I} \otimes T)CNOT(\mathbb{I} \otimes T^\dagger)(\mathbb{I} \otimes H)(\mathbb{I} \otimes S^\dagger)(|01\rangle - |10\rangle)/\sqrt{2} \\ &= (\mathbb{I} \otimes S)(\mathbb{I} \otimes H)(\mathbb{I} \otimes T)CNOT(\mathbb{I} \otimes T^\dagger)(\mathbb{I} \otimes H)(-i|01\rangle - |10\rangle)/\sqrt{2} \\ &= (\mathbb{I} \otimes S)(\mathbb{I} \otimes H)(\mathbb{I} \otimes T)CNOT(\mathbb{I} \otimes T^\dagger)(-i|00\rangle + i|01\rangle - |10\rangle - |11\rangle)/2 \\ &= (\mathbb{I} \otimes S)(\mathbb{I} \otimes H)(\mathbb{I} \otimes T)CNOT(-i|00\rangle + ie^{-i\pi/4}|01\rangle - |10\rangle - e^{-i\pi/4}|11\rangle)/2 \\ &= (\mathbb{I} \otimes S)(\mathbb{I} \otimes H)(\mathbb{I} \otimes T)(-i|00\rangle + ie^{-i\pi/4}|01\rangle - |11\rangle - e^{-i\pi/4}|10\rangle)/2 \\ &= (\mathbb{I} \otimes S)(\mathbb{I} \otimes H)\left(-i|00\rangle + i|01\rangle - e^{i\pi/4}|11\rangle - e^{-i\pi/4}|10\rangle\right)/2 \\ &= (\mathbb{I} \otimes S)(-2i|01\rangle - \sqrt{2}|10\rangle + i\sqrt{2}|11\rangle)/2\sqrt{2} \\ &= \frac{1}{\sqrt{2}}|01\rangle - \frac{1}{2}|10\rangle - \frac{1}{2}|11\rangle \end{aligned}$$

Quantum circuit

- A quantum circuit is reversible!

$$\begin{aligned}
 & (CH)^\dagger \left(\frac{1}{\sqrt{2}}|01\rangle - \frac{1}{2}|10\rangle - \frac{1}{2}|11\rangle \right) = \\
 & = (\mathbb{I} \otimes S^\dagger)(\mathbb{I} \otimes H)(\mathbb{I} \otimes T^\dagger)CNOT(\mathbb{I} \otimes T)(\mathbb{I} \otimes H)(\mathbb{I} \otimes S) \left(\frac{1}{\sqrt{2}}|01\rangle - \frac{1}{2}|10\rangle - \frac{1}{2}|11\rangle \right) = \\
 & = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle)
 \end{aligned}$$

- A quantum circuit operates in parallel!



Shor code for error correction

Transverse Ising model

Transverse Ising model

First-neighbor interaction (with Periodic Boundary Condition) with a transverse field of λ strength:

$$H = \sum_{i=1}^n \sigma_i^x \sigma_{i+1}^x + \underbrace{\sigma_n^x \sigma_1^x}_{PBC} + \lambda \sum_{i=1}^n \sigma_i^z$$

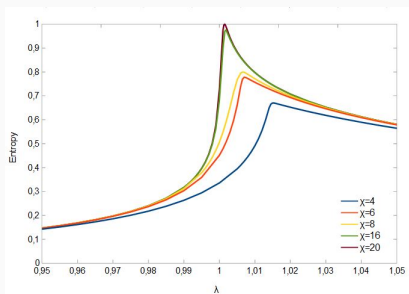
PBC term is difficult to map into fermionic operators, so we add an extra term to do the correct mapping:

$$H = \sum_{i=1}^n \sigma_i^x \sigma_{i+1}^x + \lambda \sum_{i=1}^n \sigma_i^z + \sigma_1^y \sigma_2^z \cdots \sigma_{n-1}^z \sigma_n^y$$

and we will solve the model as it was infinite: finite-size effects will appear but they become negligible as $n \rightarrow \infty$.

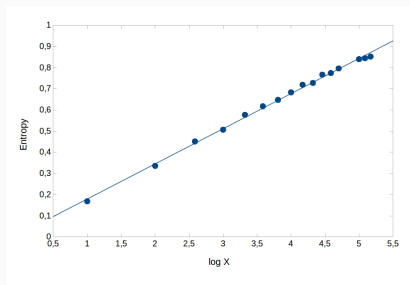
Quantum Phase Transition

Paramagnetic to ferromagnetic quantum phase transition. Entanglement entropy peaks at critical point and conformal invariance is recovered ²



$\lambda_c \rightarrow 1$ as $\chi \rightarrow \infty$: Conformal invariance

$S(\chi) \sim \frac{c}{6} \log_2 \chi$ with $c = 1/2$ for fermions.



Fit: $S(\chi) = 0.166 \log_2 \chi + 0.014$
 $\rightarrow c = 0.48(1)$

²J. I. Latorre, E. Rico, G. Vidal, Quant. Inf. Comput. 4 48-92 (2004), arXiv:quant-ph/0304098

Magnetization

Transverse magnetization: $M = \frac{\hbar}{2} \langle \sigma_z \rangle$.

Choice of computational basis $|0\rangle = |\uparrow\rangle$, $|1\rangle = |\downarrow\rangle$:

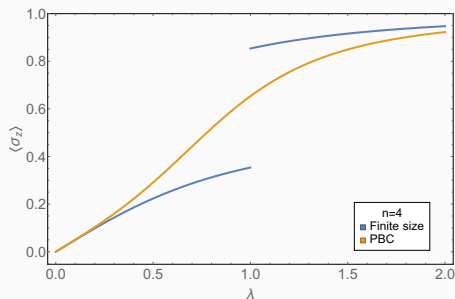
$$\begin{aligned}\sigma_z |\uparrow\rangle &= +1 |\uparrow\rangle \\ \sigma_z |\downarrow\rangle &= -1 |\downarrow\rangle\end{aligned}$$

$$\langle \sigma_z \rangle = \frac{1}{n} \sum_{i=1}^{2^n} p_i \langle e_i | \sigma_z | e_i \rangle = \frac{1}{n} \sum_{i=1}^{2^n} p_i (n_i^0 - n_i^1) = \frac{1}{n} \sum_{i=1}^{2^n} p_i (n - 2n_i^1)$$

$$|\psi\rangle = \sum_{i=1}^{2^n} p_i |e_i\rangle$$

$|e_i\rangle$ computational basis states

$n_i^0(n_i^1)$ n^o of $|0\rangle(|1\rangle)$



Solving the Transverse Ising Model ³ ⁴

³E. Lieb, T. Schultz, D. Mattis, Annals of Physics **16**, Issue 3, 407-466 (1961)

⁴S. Katsura, Phys. Rev. **127**, 1508 (1962)

Jordan-Wigner transformation

Maps the spin operators into fermionic modes:

$$c_j = \left(\prod_{m < j} \sigma_m^z \right) \frac{\sigma_j^x - i\sigma_j^y}{2}, \quad c_j^\dagger = \left(\prod_{m < j} \sigma_m^z \right) \frac{\sigma_j^x + i\sigma_j^y}{2}$$

$$\{c_i, c_j\} = 0, \quad \{c_i, c_j^\dagger\} = \delta_{ij}, \quad c_i |\Omega_c\rangle = 0$$

$$H_c = \frac{1}{2} \sum_{i=1}^n \left(c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1} + c_i^\dagger c_{i+1}^\dagger + c_i c_{i+1} \right) + \lambda \sum_{i=1}^n c_i^\dagger c_i$$

In terms of the wave function

$$|\Psi\rangle = \sum_{\{i_n\}=0}^1 \psi_{i_1, i_2, \dots, i_n} |i_1, i_2, \dots, i_n\rangle \xrightarrow{J.W.} |\Psi\rangle_c = \sum_{\{i_n\}=0}^1 \psi_{i_1, i_2, \dots, i_n} (c_1^\dagger)^{i_1} (c_2^\dagger)^{i_2} \dots (c_n^\dagger)^{i_n} |\Omega_c\rangle$$

→ Wave function coefficients do not change!

No need of implementing any operation in the circuit!

Fourier transform

Exploits translational invariance and takes H_c into a momentum space hamiltonian H_b :

$$b_k = \frac{1}{\sqrt{n}} \sum_{j=1}^n e^{i\frac{2\pi}{n}jk} c_j, \quad b_k^\dagger = \frac{1}{\sqrt{n}} \sum_{j=1}^n e^{-i\frac{2\pi}{n}jk} c_j^\dagger, \quad k = -\frac{n}{2} + 1, \dots, \frac{n}{2}$$

$$H_b = \sum_{k=0}^{n-1} \left[2 \left(\lambda - \cos \left(\frac{2\pi k}{n} \right) \right) b_k^\dagger b_k + i \sin \left(\frac{2\pi k}{n} \right) \left(b_{-k}^\dagger b_k^\dagger + b_{-k} b_k \right) \right]$$

If $n = 2^m$, we can implement the Fast Fourier Transform (more efficient)

$$\frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} e^{i\frac{2\pi}{n}jk} c_j = \frac{1}{\sqrt{n/2}} \sum_{j'=0}^{n/2-1} e^{i\frac{2\pi}{n/2}j'k} c_{2j'} + \frac{e^{i\frac{2\pi k}{n}}}{\sqrt{n/2}} \sum_{j'=0}^{n/2-1} e^{i\frac{2\pi}{n/2}j'k} c_{2j'+1}$$

$$b_k \equiv \frac{1}{\sqrt{2}} \left(b_{k_{\text{even}}} + e^{i\frac{2\pi k}{n}} b_{k_{\text{odd}}} \right), \quad b_k^\dagger \equiv \frac{1}{\sqrt{2}} \left(b_{k_{\text{even}}}^\dagger + e^{i\frac{2\pi k}{n}} b_{k_{\text{odd}}}^\dagger \right)$$

Bogoliubov transformation

Decouples the modes with opposite momentum. For the Ising model

$$\begin{aligned}a_k &= \cos\left(\frac{\theta_k}{2}\right) b_k - i \sin\left(\frac{\theta_k}{2}\right) b_{-k}^\dagger \\a_k^\dagger &= \cos\left(\frac{\theta_k}{2}\right) b_k^\dagger + i \sin\left(\frac{\theta_k}{2}\right) b_{-k}\end{aligned}$$

where $\theta_k = -\arccos\left(\frac{\lambda - \cos\left(\frac{2\pi k}{n}\right)}{\sqrt{(\lambda - \cos\left(\frac{2\pi k}{n}\right))^2 + \sin^2\left(\frac{2\pi k}{n}\right)}}\right)$

$$\boxed{H_a = \sum_k \omega_k a_k^\dagger a_k} \quad \omega_k = \sqrt{\left(\lambda - \cos\left(\frac{2\pi k}{n}\right)\right)^2 + \sin^2\left(\frac{2\pi k}{n}\right)}$$

Ground state energy: $\epsilon_0 = -\sum_k \omega_k$

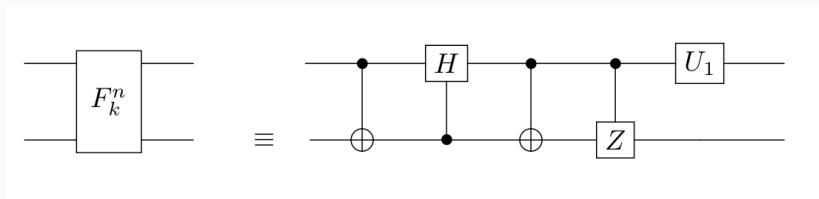
Implementation

2-qubit quantum gates

Fourier transform⁵

$$F_k^n = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{e^{-\frac{2\pi i k}{n}}}{\sqrt{2}} & -\frac{e^{-\frac{2\pi i k}{n}}}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & -e^{-\frac{2\pi i k}{n}} \end{pmatrix}$$

$$U_1 = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$$



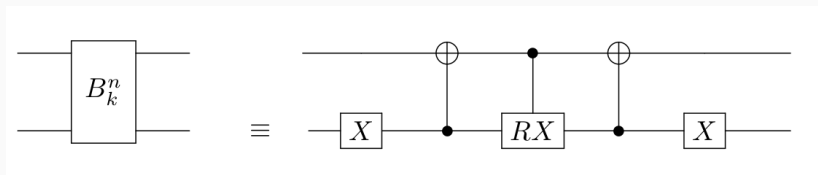
⁵A. J. Ferris, Phys. Rev. Lett. **113**, 010401 (2014), arXiv:quant-ph/1310.7605

2-qubit quantum gates

Bogoliubov transformation

$$B_k^n = \begin{pmatrix} \cos\left(\frac{\theta_k}{2}\right) & 0 & 0 & i \sin\left(\frac{\theta_k}{2}\right) \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ i \sin\left(\frac{\theta_k}{2}\right) & 0 & 0 & \cos\left(\frac{\theta_k}{2}\right) \end{pmatrix}$$

$$RX = \begin{pmatrix} \cos(\theta/2) & i \sin(\theta/2) \\ i \sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

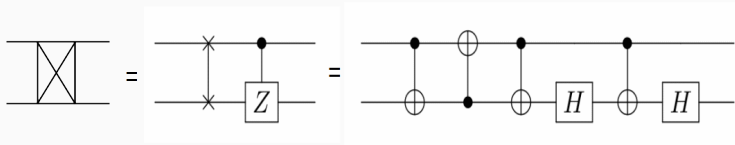


2-qubit quantum gates

Fermionic SWAP

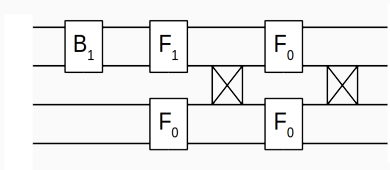
SWAP gate exchange the qubits state, *i.e.* maps $|01\rangle \leftrightarrow |10\rangle$. But due to the anticommutation relations of fermions, if two occupied modes exchange, they must carry a minus sign:

$$fSWAP = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

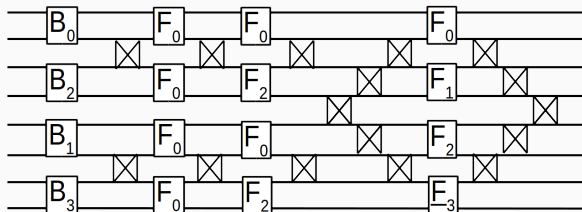


$$\tilde{H} \equiv H_a \xrightarrow{U_{Bog}} H_b \xrightarrow{U_{FT}} H_c \longrightarrow H \implies U_{dis} = U_{FT} U_{Bog} \quad ^6$$

$n = 4$

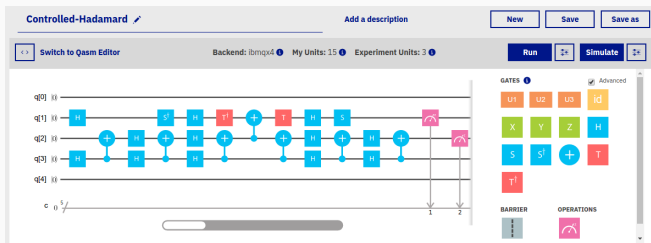


$n = 8$



⁶F. Verstraete, J. I. Cirac, J. I. Latorre, Phys. Rev. A **79**, 032316 (2009),
arXiv:quant-ph/0804.1888

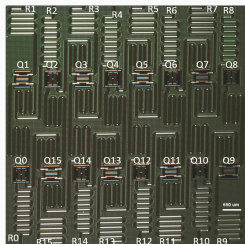
- **Cloud Quantum Computation:** IBM Q experience⁷ and Quantum Information Software Kit (QISKit)⁸
- **Platform:** Superconducting transmon qubits
- **Devices:** ibmqx2 (5 qubits), ibmqx4 (5 qubits), **ibmqx5 (16 qubits)**
- **Gate set:** $CNOT$, U_1 , U_2 , U_3 , H , X , Y , Z , S , S^\dagger , T , T^\dagger



⁷<http://ibm.quantumexperience.ng.bluemix.net>

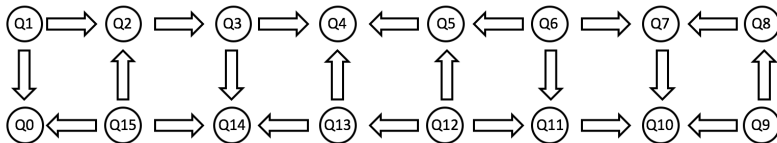
⁸<http://qiskit.org> and <http://github.com/QISKit>

ibmqx5: Albatross

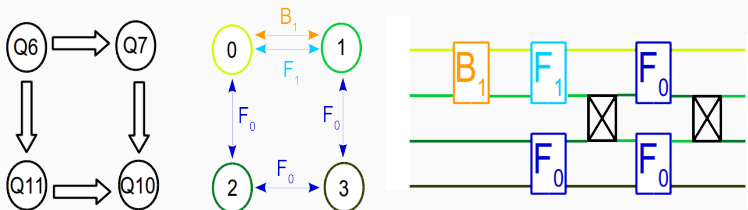


- 16 superconducting transmon qubits
(a kind of charge qubit: eigenstates represent the presence or absence of excess Cooper pairs)
- Relaxation time: $T_1 = 30 - 50\mu s$
- Coherence time: $T_2 = 30 - 90\mu s$
- Gate pulses: $CNOT \sim 550 - 800ns$, $U_3 \sim 160ns$
- Gate error (10^{-2}): 0.2 – 0.4 (1Q), 4 – 10 (readout), 3 – 10 (2Q)

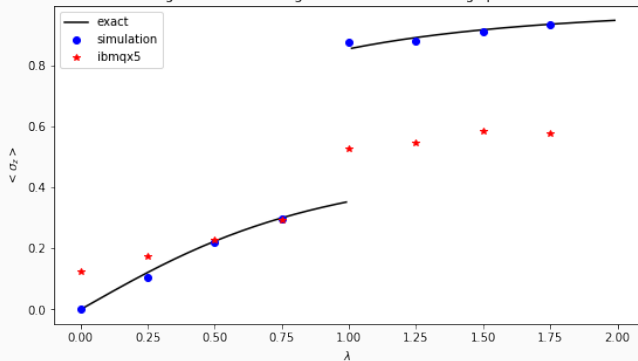
Topology/architecture: Control \Rightarrow target



Results $n = 4$



Magnetization of the ground state of $n=4$ Ising spin chain



Time evolution

Time evolution operator

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle \xrightarrow{H \neq H(t)} |\Psi(t)\rangle = U(t) |\Psi_0\rangle, \quad \boxed{U(t) = e^{-itH}}$$

$$|\Psi(t)\rangle = \sum_n e^{-itE_n} |E_n\rangle \langle E_n | \Psi_0\rangle$$

$$\langle \Psi(t) | \mathcal{O} | \Psi(t) \rangle = \sum_n \sum_m e^{-it(E_n - E_m)} \langle \Psi_0 | E_m \rangle \langle E_m | \mathcal{O} | E_n \rangle \langle E_n | \Psi_0 \rangle$$

If $[H, \mathcal{O}] \neq 0$ and $|\Psi_0\rangle$ is not an stationary state, we can observe an oscillation with t with phase $(E_n - E_m)$.

1. Choose $|\Psi_0\rangle$ written in terms of the \tilde{H} basis: $|\Psi_0\rangle = \sum_i c_i |\psi_i\rangle$
2. Apply time-evolution operator:
 $|\Psi(t)\rangle = e^{-it\tilde{H}} |\Psi_0\rangle = \sum_i c_i e^{-it\epsilon_i} |\psi_i\rangle$
3. Implement the U_{dis} gate to transform the state into the Ising basis:

$$\boxed{|\Phi(t)\rangle = U_{dis} |\Psi(t)\rangle = U_{dis} \sum_i c_i e^{-it\epsilon_i} |\psi_i\rangle}$$

Time evolution | ↑↑↑↑> state

$|\varphi_0\rangle = |\uparrow\uparrow\uparrow\uparrow\rangle \equiv |0000\rangle_{Is}$ in the Ising basis:

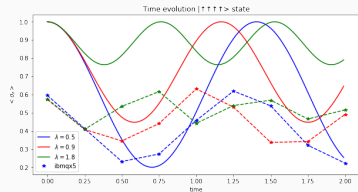
$$|\psi_0\rangle = U_{dis}^\dagger |0000\rangle_{Is} = \cos \phi |0000\rangle + i \sin \phi |1100\rangle,$$

with $\phi = \frac{1}{2} \arccos\left(\frac{\lambda}{\sqrt{1+\lambda^2}}\right)$.

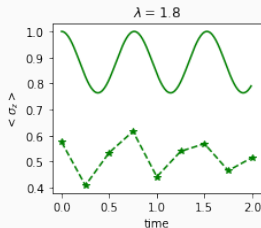
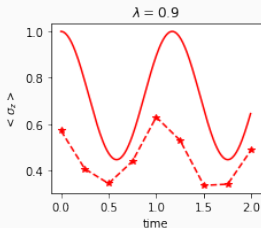
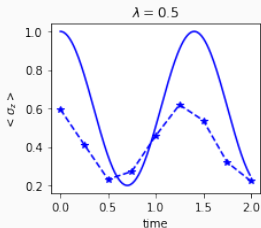
Time evolution: add the corresponding phases

$e^{-it\epsilon_i}$ where ϵ_i are the energies of the states $|0000\rangle$

and $|1100\rangle$:



$$|\psi(t)\rangle \propto (\cos \phi |00\rangle + i e^{4it\sqrt{1+\lambda^2}} \sin \phi |11\rangle) \otimes |00\rangle \rightarrow |\varphi(t)\rangle = U_{dis} |\psi(t)\rangle$$



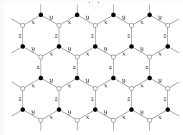
Other models

Other models

Other exactly-solvable models:

- XY model:

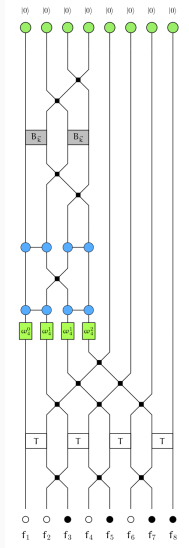
$$H_{XY} = \sum_{i=1}^n \left(\frac{1+\gamma}{2} \sigma_i^x \sigma_{i+1}^x + \frac{1-\gamma}{2} \sigma_i^y \sigma_{i+1}^y \right) + \lambda \sum_{i=1}^n \sigma_i^z$$



- Kitaev-Honeycomb model⁹

$$H = -J_x \sum_{x\text{-links}} \sigma_i^x \sigma_j^x - J_y \sum_{y\text{-links}} \sigma_i^y \sigma_j^y - J_z \sum_{z\text{-links}} \sigma_i^z \sigma_j^z$$

Heisenberg Model: *Bethe Ansatz*?



⁹P. Scholl, R. Orús, Phys. Rev. B **95**, 045112 (2017), arXiv:cond-mat/1605.04315

Summary

Summary

- It is possible to design an efficient quantum circuit that solves *exactly* integrable hamiltonians
- Available quantum computers such as IBM Q can implement these circuits and simulate few qubit systems
- Example, $n = 4$ Ising spin chain circuit: magnetization for $\lambda < 1$ is well simulated and for $\lambda > 1$ catches the correct trend as well as time evolution for different λ
- Still high error rates and low T_1 and T_2 to simulate larger systems

This has been an example of how to program a quantum computer to simulate a spin chain:

→ **Useful to test quantum computers**

→ **Can we apply what we have learned to simulate non integrable models?**

Thanks!