

Quantum Simulation of The Transverse Ising Model

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We present a simulation of transverse Ising model using the QISKIT. The main goal is to find the ground state of such system. Two ways had been used. First, the variational eigenvalue solver with local simulator. Second, the direct diagonalization of the Hamiltonian. All, the results had been compared with each other under the conditions of four spins and the periodic boundary condition.

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Introduction



The problem encountered

1. Novel properties are found in material which involves strong quantum correlation between electrons.
2. The Hilbert space has dimension of $O(2^n)$, which is unsolvable with classical computer in the foreseeable future.
3. Sign problem or some other problem still occur for many models and methods.
4. We try to solve this problem by some basic quantum circuits combining with classical algorithms.

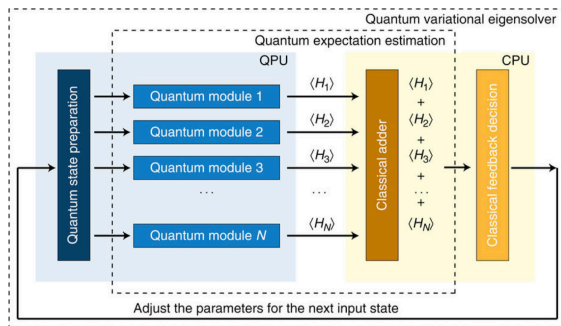
Variational quantum eigenvalue solver

$$\mathcal{H} |\psi\rangle = E_g |\psi\rangle \quad (1)$$

In this report, we experiment with IBM local quantum simulator by searching the ground state energy of the transverse Ising model and the corresponding best ansatz for ground state. The actual device is not used for the sake of communication bottleneck.

Variational quantum eigenvalue solve

Quantum phase estimation algorithm is a choice. However, it involves the inverse quantum fourier transformation, which takes too many gates and too much gate time for current achievable coherent time. To face these problems, we use the variational quantum eigenvalue solver (VQES)[1].



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Variational quantum eigenvalue solve: The procedure

1. Prepare a variational ansatz state $|\psi(\theta_i)\rangle$ with parameters θ_i . To be efficient, parameters should grow with system size linearly.
2. Calculate the expectation value of energy using quantum computer $E = \langle \psi | \mathcal{H} | \psi \rangle / \langle \psi | \psi \rangle$
3. By classical algorithm, determining a new optimal θ_i which minimize the energy.
4. Iterate the above until convergence.

The System Considered

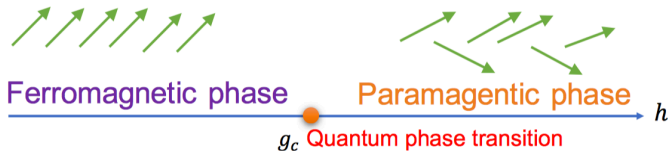
The Transverse Ising Model

We consider the transverse Ising model (TIM):

$$\mathcal{H} = - \sum_i \sigma_i^z \sigma_{i+1}^z - h \sum_i \sigma_i^x, \quad (2)$$

σ^z, σ^x are Pauli matrices and h is the relative transverse field strength. First, notice that the Hamiltonian is invariant under rotation along x axis by π , $R_x \mathcal{H} R_x^\dagger = \mathcal{H}$, since,

$$R_x \sigma^x R_x^\dagger = \sigma^x, R_x \sigma^z R_x^\dagger = -\sigma^z \quad (3)$$



(Fig2) Schematic view of the quantum phases described by the transverse Ising model. The arrows represent the spin configuration in the ordered and disordered phases.

TIM has two phase (Fig2): When h is small, the x rotation symmetry is broken. $\langle \sigma^z \rangle \neq 0$. With h grows, $\langle \sigma^z \rangle = 0$.

Since there are ordered and disordered phase, we may try the following trial state which rotate each spin:

$$|\psi_i(\theta_i)\rangle = \prod_i U(\theta_i) |0_i\rangle \quad (4)$$

$$U(\theta_i) = \begin{pmatrix} \cos(\theta_i/2) & -\sin(\theta_i/2) \\ \sin(\theta_i/2) & \cos(\theta_i/2) \end{pmatrix} \quad (5)$$

Method



The expectation value is calculated by,

$$E_{J,i} = -\langle \psi | \sigma_i^z \sigma_{i+1}^z | \psi \rangle, E_{Z,i} = -\langle \psi | \sigma_i^x | \psi \rangle \quad (6)$$

By simple calculation, we can see:

$$E_{J,i} = -[P(q_i = 0) - P(q_i = 1)][P(q_{i+1} = 0) - P(q_{i+1} = 1)] \quad (7)$$

$$E_{Z,i} = -[P(q_i = 0) - P(q_i = 1)] \quad (8)$$

$$(9)$$

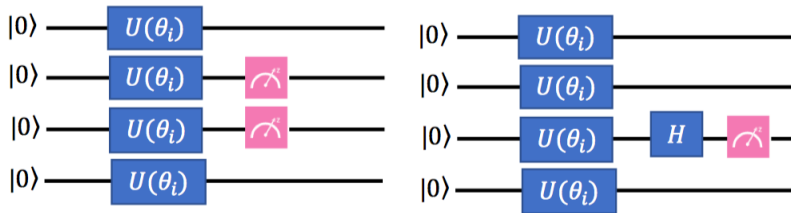
Let $\psi = a |0\rangle + b |1\rangle$,

$$H(\text{Hadamard}) |\psi\rangle = \frac{1}{\sqrt{2}} ((a + b) |0\rangle + (a - b) |1\rangle) \quad (10)$$

$$P(q_i = 0) - P(q_i = 1) = a^*b + b^*a \quad (11)$$

$$= \langle \sigma^x \rangle \quad (12)$$

Therefore, the circuits in (Fig3) serve the purpose.

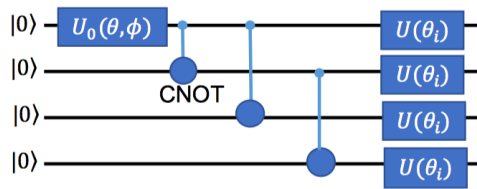


(Fig3) Left $\langle \sigma_i^z \sigma_{i+1}^z \rangle$, Right $\langle \sigma_i^x \rangle$

We know that entanglement plays an important roll in such system, but the previous trial state has no entanglement. Also, for the sake of symmetry, if $|\psi_i\rangle$ is a eigenstate, $R_x(\pi) |\psi_i\rangle$ is also one. We try to have:

$$|\psi'_i(\theta_i)\rangle = \alpha |\psi_i(\theta_i)\rangle + \beta R_x(\pi) |\psi_i(\theta_i)\rangle \quad (13)$$

The following circuit serves our purpose:



(Fig4) Circuit for trial state 2

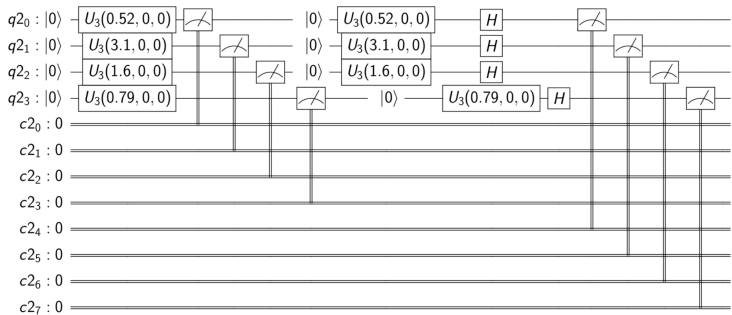
The U_0 and the CNOTs transform the state into:

$$e^{i\phi} \sin(\theta/2) |1111\rangle + \cos(\theta/2) |0000\rangle \quad (14)$$

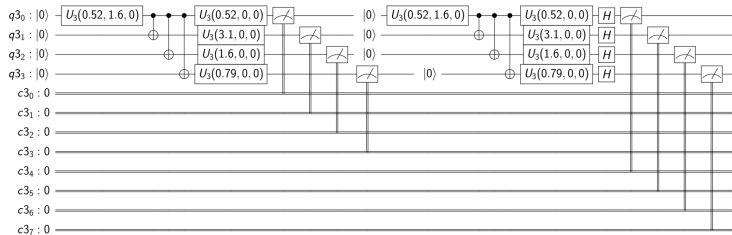
Since the final four U_0 transform $|0000\rangle$ into $|\phi\rangle$, we attain our goal. Here,

$$U_0(\theta, \phi) = \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ e^{i\phi} \sin(\theta/2) & e^{i\phi} \cos(\theta/2) \end{pmatrix}$$

The QISKIT local simulator was used for $N = 4$ four qubit system. The shot was set 1024. The circuits are the following with a randomly choose θ , θ_i and ϕ . The θ_i is the searching space to be optimized.



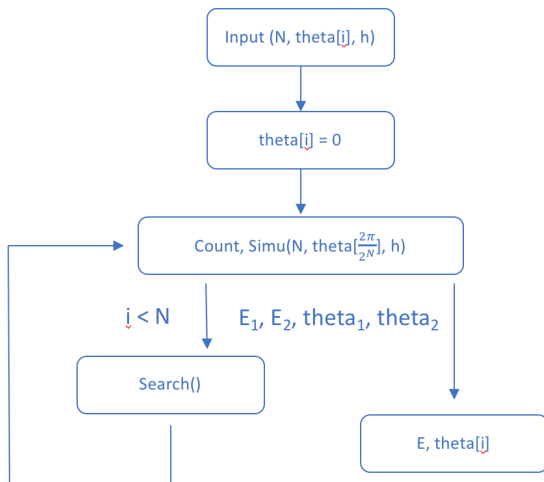
(Fig5) Circuit in used for the first initial condition



(Fig6) Circuit in used for the second initial condition

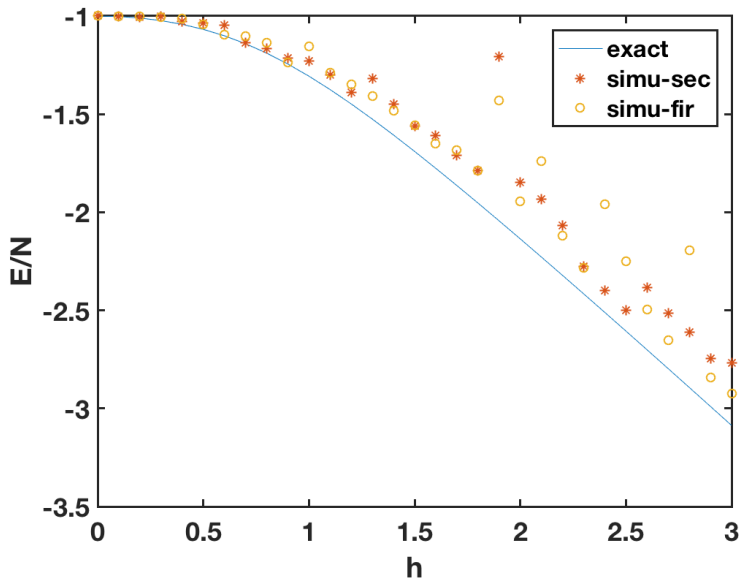
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Classical optimized algorithm



Result and discussion

Result





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The second initial condition gives better approximation to the exact solution, because in this case the entanglement is considered. Also, the main advantage of the second one is on the region where h is bigger. This makes sense because this correspond to ordered phase and entanglement get more involved in the ordered phase. Generally, the simulated energy is bigger than exact one, this part of error might came from the efficiency of classical search algorithm.

The merits of this model is efficiency. However, the cpu and qpu must be near each other so as to overcome the communication bottlenec at this point. But, quantum communication maybe use to overcome the bottleneck. This method is a promising way to solve CMT problem. In the near future, 100 qubits quatum computer can be realized and test many current high temperature superconduting model.

Reference

-  Alberto Peruzzo, Jarrod McClean, Peter Shadbolt, Man-Hong Yung, Xiao-Qi Zhou, Peter J. Love, Alan Aspuru-Guzik, and Jeremy L. O' Brien. A variational eigenvalue solver on a photonic quantum processor. Nature Communications, 5:ncomms5213, July 2014.
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