A Quantum Algorithm for a Classical Spin Model

Project for the exam of Quantum Computing

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We will present an efficient quantum algorithms to estimate the partition function $\mathcal{Z}$ of the Ising model on a planar graph with magnetic fields. The result is proven for a complex parameter regime. The algorithm is based on a mapping relating partition functions to quantum circuits. One can show that this problem is BQP-complete.

1 Theoretical introduction

1.1 2D Ising model with fields

We will consider a 2-dimensional classical Ising model with a planar square lattice of size n. This model can be described as an edge model, so consider a graph G with vertex set V and edge set E (Fig. 1). We associate a 2-level classical spin variable $s_i \in \{0, 1\}$ to each vertex $i \in V$ of the lattice. Let $\vec{s}$ denote the set of all the values of the spin variables. To each edge $e = (i, j) \in E$ of the lattice we associate a spin-spin interaction, which is a 2-body interaction described by $h_e(s_i, s_j) = -J_e\delta(s_i + s_j)$, where the sum $s_i + s_j$ is modulo 2, while

$$\delta(x) = \begin{cases} 1 & \text{if } x = 0 \\ 0 & \text{otherwise} \end{cases}.$$

We will also consider an external magnetic field $h_i(s_i) = -h_i\delta(s_i)$ at each site i of the lattice.
The full Hamiltonian of the system is given by

$$H(\vec{s}) = -\sum_{e=(i,j)\in E} J_e\delta(s_i + s_j) - \sum_{i\in V} h_i\delta(s_i).$$

Let β denote the inverse of the temperature. Given these interactions, the corresponding Boltzmann factor for the edge e (spin-spin interaction) is

$$w_e(s_i, s_j) = e^{-\beta h_e(s_i,s_j)},$$

whereas for the vertex i (spin-magnetic field interaction) we have

$$w_i(s_i) = e^{-\beta h_i(s_i)}.$$

The complete partition function of this model is given by

$$\mathcal{Z} = \sum_{\vec{s}} e^{-\beta H(\vec{s})},$$

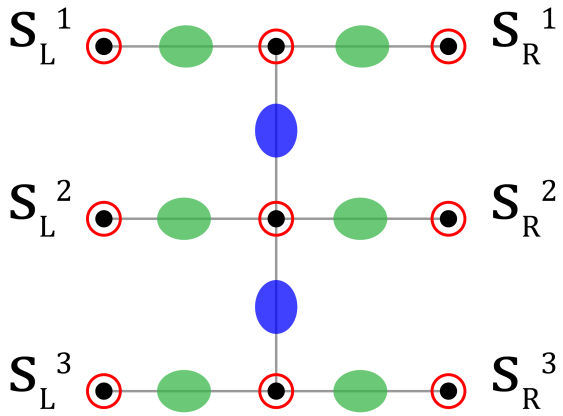


Figure 1: The graph G of the lattice for $n = 3$. The black circles represent the vertices (so the spin variables) and the red circles are the corresponding spin-magnetic field interactions, the grey lines are the edges and the corresponding ovals are the spin-spin interactions (blue in the vertical direction and green in the horizontal one). The boundary conditions are also represented, on the right $R = (s_R^1, s_R^2, s_R^3)$ and on the left $L = (s_L^1, s_L^2, s_L^3)$.

or, in terms of the Boltzmann factors w_e and w_i:

$$\mathcal{Z} = \sum_{\vec{s}} \prod_{e=(i,j)\in E} \prod_{k\in V} w_e(s_i, s_j) w_k(s_k).$$

The goal of this project is to estimate this partition function using a quantum circuit.

1.2 Lattice - Circuit Map

The partition function $\mathcal{Z}$ of a classical spin model, as the Ising one, on a certain complex parameter regime can be approximated efficiently by quantum algorithms with polynomial accuracy.
Consider our square lattice, so that one direction can be associated to time, for instance the horizontal one. We will relate the partition function $\mathcal{Z}$ to a quantum circuit $\mathcal{C}$ by mapping variables in the classical model to the time evolution of qubits in the circuit. Additionally, each interaction will be mapped to a quantum gate; more precisely, the entries of the quantum gate will be given by the Boltzmann weights of the corresponding interaction. Then, the product of interactions in $\mathcal{Z}$ will be mapped to the contraction of gates in $\mathcal{C}$. This map between the classical lattice and the quantum circuit $\mathcal{C}$ will allow us to interpret the partition function $\mathcal{Z}$ of the classical model as a quantum expectation value.
For an edge model, as the Ising model, we shall distinguish between interactions at horizontal (time) and vertical edges. If $e = (i, j)$ is along the horizontal (time) direction, we map it to a single-qubit gate:

$$W_e^h = \sum_{s_i, s_j} w_e(s_i, s_j) \left|s_j\right\rangle \left\langle s_i\right|,$$

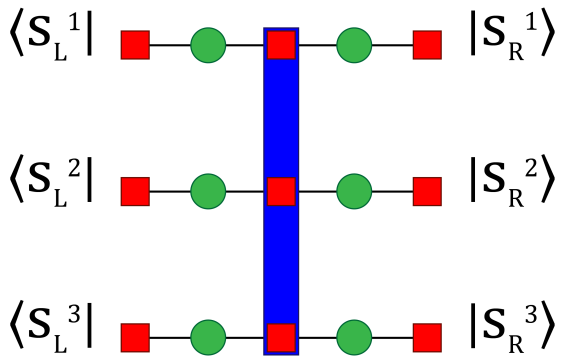


Figure 2: The circuit $\mathcal{C}$ associated to the lattice (Fig. 1) for $n = 3$. The red squares represent the V single-qubit gates, the green circles are the $\bar{W}_h$ single-qubit gates and the blue rectangles are the W_v two-qubit gates. The boundary conditions are also represented, on the right $|R\rangle = \left|s_R^1\right\rangle \otimes \left|s_R^2\right\rangle \otimes \left|s_R^3\right\rangle$ and on the left $|L\rangle = \left|s_L^1\right\rangle \otimes \left|s_L^2\right\rangle \otimes \left|s_L^3\right\rangle$.

whereas if $e = (i, j)$ is along the vertical direction, we map it to a diagonal two-qubit gate:

$$W_e^v = \sum_{s_i, s_j} w_e(s_i, s_j) \left|s_i s_j\right\rangle \left\langle s_i s_j\right| .$$

Finally we map a vertex i coupled to the magnetic field to the diagonal single-qubit gate:

$$W_i = \sum_{s_i} w_i(s_i) \left|s_i\right\rangle \left\langle s_i\right| .$$

With the definitions of the Boltzmann factors, w_e and w_i, given before, these gates can be written as the following operators:

$$W_e^h = \begin{pmatrix} e^{\beta J_e} & 1 \\ 1 & e^{\beta J_e} \end{pmatrix},$$

$$W_e^v = \begin{pmatrix} e^{\beta J_e} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{\beta J_e} \end{pmatrix},$$

$$W_i = \begin{pmatrix} e^{\beta h_i} & 0 \\ 0 & 1 \end{pmatrix}.$$

Recall that n is the number of vertex both in the horizontal and vertical direction. In this way the associated circuit $\mathcal{C}$ is an n–qubit circuit composed of layers of the gates W_e^h, W_e^v and W_i (Fig. 2).

Note that the three previous operators to be unitary, and so to be well-defined quantum gates, they need complex coupling strengths J_e and h_i.

Finally let us discuss the map of the boundary conditions. If the spin model has fixed boundary conditions on the right $R = (s_R^1, ..., s_R^n)$ and on the left $L = (s_L^1, ..., s_L^n)$, these are mapped to the input $|R\rangle = \left|s_R^1\right\rangle \otimes ... \otimes \left|s_R^n\right\rangle$ and output $|L\rangle = \left|s_L^1\right\rangle \otimes ... \otimes \left|s_L^n\right\rangle$ of the circuit. One can verify the following correspondence

$$\mathcal{Z}_{R,L} = \langle L| \mathcal{C} |R\rangle .$$

Whereas for open boundary conditions (OBC) we have

$$\mathcal{Z}_{OBC} = 2^n \langle +|^{\otimes n} \mathcal{C} |+\rangle^{\otimes n},$$

where the state $|+\rangle$ is defined by

$$|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}.$$

For periodic boundary conditions (PBC) the partition function is

$$\mathcal{Z}_{PBC} = \mathrm{Tr}\{\mathcal{C}\}.$$

1.3 Complex coupling strengths

Now we will take a particular choice of the coupling strengths J_e and h_i for which we can give an efficient quantum algorithms to estimate the partition function $\mathcal{Z}$. We require that the magnetic couplings h_i on each vertex i is complex and satisfies

$$e^{\beta h_i} = e^{i\pi/4},$$

whereas the spin couplings J_e on each edge e satisfies

$$e^{\beta J_e} = i.$$

Gates corresponding to this model are of the form:

$$W_h = \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix},$$

$$W_v = \begin{pmatrix} i & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & i \end{pmatrix},$$

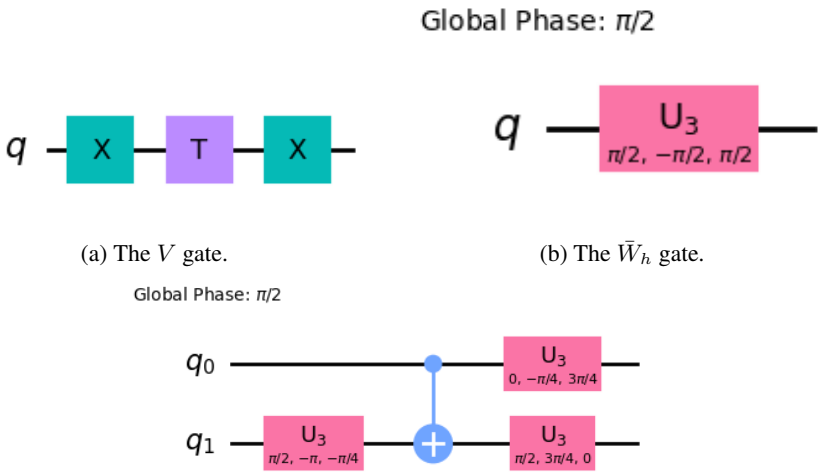
$$V = \begin{pmatrix} e^{i\pi/4} & 0 \\ 0 & 1 \end{pmatrix}.$$

Where $W_i = V$, and we removed the dependence on the edge e and the vertex i because the interactions are homogeneous.
The matrices W_v and V are unitary. Moreover, the matrix $\bar{W}_h = W_h/\sqrt{2}$ is unitary as well. Letting $\bar{\mathcal{C}}$ denote the unitary quantum circuit obtained by replacing every gate W_h by $\bar{W}_h$, we simply have $\bar{\mathcal{C}} = 2^{-\tau/2}\mathcal{C}$, where τ is the number of W_h presents in $\mathcal{C}$ (and so the number of horizontal edges in the lattice).

2 Quantum Circuit

2.1 Implementation of the circuit

For the implementation of the quantum circuit we use the software Qiskit.
First we define the operators $\bar{W}_h$, W_v and V using the class `Operator` and their matrix representation (Fig. 3).
The quantum circuit $\mathcal{C}$ consists of n-qubits and it is the result of the application of layers



(a) The V gate.

(b) The $\bar{W}_h$ gate.

(c) The W_v gate.

Figure 3: The gates representing the interaction in the lattice.

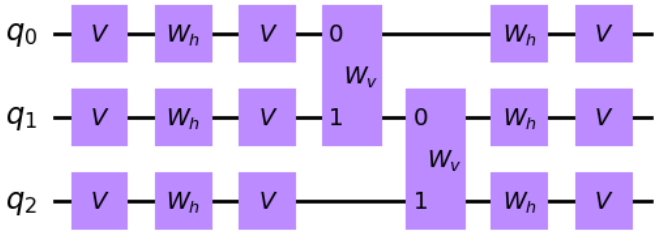


Figure 4: The quantum circuit for $n = 3$.

of the gates $\bar{W}_h$, W_v and V (Fig. 4). We construct it using the class `QuantumCircuit`. We create the different input states using the class `Statevector` for different boundary conditions: $|R\rangle$ for R, L and $|+\rangle^{\otimes n}$ for OBC. Then we make them evolve according to the quantum circuit, using the method `evolve()`. Finally using the method `inner()` we compute the scalar product with the output states: $|L\rangle$ for R, L and $|+\rangle^{\otimes n}$ for OBC. In this way we get the partition function.

2.2 Swap Test

In a real experiment we have no access to which are the exact quantum states after the evolution in a quantum circuit or the scalar product between two of them. The swap test is a way in which we can estimate the modulus of the scalar product between two arbitrary states by measuring the probability p_0 of getting 0 on an ancilla qubit.
In the swap test quantum circuit there are three input states, the first one is an ancilla qubit initialize to $|0\rangle$, the second one is the state $\bar{\mathcal{C}}\,|R\rangle$ represented by n qubits, and the third one is the state $|L\rangle$ represented by n qubits. We have to apply an Hadamard gate

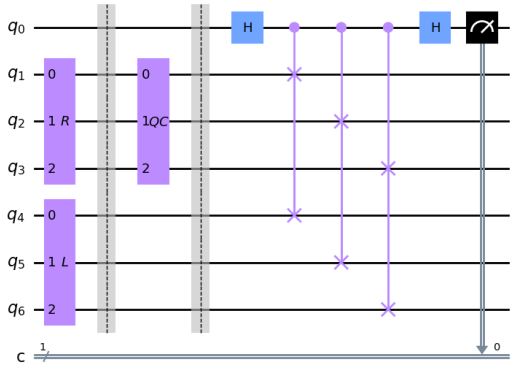


Figure 5: The quantum circuit for the evaluation of $|\mathcal{Z}_{L,R}|$ with a swap test for $n = 3$. The gate R initialize three qubits to $|R\rangle$, the gate L initialize three qubits to $|L\rangle$. The gate QC is the quantum circuit represented in (Fig. 4).

to the first qubit, a controlled swap between the other two states, and then an Hadamard to the first qubit. (Fig. 5)

Measuring the ancilla qubit and the frequency p_0 with which it is found in the state $|0\rangle$, we are able to estimate the modulus square of the scalar product between the states $\bar{C}\,|R\rangle$ and $|L\rangle$, strictly related to $|\mathcal{Z}_{L,R}|^2$. Indeed we have

$$|\mathcal{Z}_{L,R}|^2 = 2^\tau (2p_0 - 1).$$

2.3 Results

In this section we summarize some of the numerical results that we obtained from Qiskit simulations.

In the next table we collect the results for the partition functions $\mathcal{Z}$ for three different boundary conditions (left and right fixed, OBC and PBC) calculated for different lattice size n by a simulation of the quantum circuit (Fig. 2) and evaluating the scalar product between two states with the method `inner()`.

n	$\mathcal{Z}_{L,R}$	$\mathcal{Z}_{OBC}$	$\mathcal{Z}_{PBC}$
2	-1.0000+0.0000j	-5.6569+2.0000j	-0.0000-2.0000j
3	3.0000+0.4142j	-44.0833-22.1421j	-5.1716-6.8284j
4	-0.6863-27.3137j	29.2548+210.7452j	-61.2548-109.2548j
5	-325.588-168.000j	-17930.106+4871.765j	-2389.410+833.332j

In the second table we collect the results for a classical combinatoric calculation of the partition function for open boundary conditions $\mathcal{Z}^{cl}_{OBC}$. Notice how these values are exactly the ones find by simulating the quantum circuit $\mathcal{Z}_{OBC}$, the algorithm seems to work. The results $|\mathcal{Z}^{swap}_{L,R}|$ represent the modulus of the partition function for left and right fixed boundary conditions calculated simulating the swap test circuit (Fig. 5) with 10000 shots. Finally $e^{swap}_{L,R}$ represents the percentage error of $|\mathcal{Z}^{swap}_{L,R}|$ with respect to $|\mathcal{Z}_{L,R}|$. More explicitly

$$e^{swap}_{L,R} = \frac{||\mathcal{Z}^{swap}_{L,R}| - |\mathcal{Z}_{L,R}||}{|\mathcal{Z}_{L,R}|} 100.$$

n	$\mathcal{Z}_{OBC}^{cl}$	$\lvert\mathcal{Z}_{L,R}^{swap}\rvert$	$e_{L,R}^{swap}$
2	-5.6569+2.0000j	1.0288	2.8786
3	-44.0833-22.1421j	2.8711	5.1961
4	29.2548+210.7452j	28.0872	2.7994
5	-17930.106+4871.765j	355.610	2.9386

We also try to run the swap test circuit (Fig. 5) for $n = 2$ on an actual quantum computer. Using the `ibm_oslo` compute resource and performing 10000 shots we get $|\mathcal{Z}_{L,R}^{swap}| = 0.8085$ with a percentage error $e_{L,R}^{swap} = 19.1545$, while using `ibmq_manila` compute resource and performing 10000 shots we get $|\mathcal{Z}_{L,R}^{swap}| = 00.9317$ with a percentage error $e_{L,R}^{swap} = 6.8335$.

3 Completeness

3.1 Notion of completeness

The question now is: why should it be interesting to calculate the partition function of a system of classical spins with complex (and non-physical) coupling constants? The answer to this question is connected with the notion of completeness.
Consider a target model with partition function $\mathcal{Z}_{G'}(J')$, defined on the graph G' and with couplings J', and another model with partition function $\mathcal{Z}_G(J)$ defined on a graph G and with couplings J. The latter model is complete if for any target, there exists a choice of couplings J and a large enough G such that $\mathcal{Z}_{G'}(J') = \mathcal{Z}_G(J)$.
It is possible to prove that the partition function of any classical spin model (target model) can be mapped to the partition function of a specific model (complete model) which is larger in size, and whose parameters specify the target model. This means that the complete model contains all other models in its parameter regime. The enlargement of complete model is polynomial with respect to the number of parameters of the target.

3.2 BQP-completeness

Classically the evaluation of the partition function is a counting problem of the complexity class #P (sharp-P). The quantum complexity class which will be considered is the "bounded-error quantum polynomial time"(BQP), representing the class of decision problems which can be solved efficiently on a quantum computer.
One can show that the problem of estimating the partition function $\mathcal{Z}$ of the Ising model with open boundary conditions, with the complex coupling strengths seen before and with polynomial accuracy is of the complexity class BQP. This problem is also known to be BQP–complete. This means that every problem in the class BQP can be reduced, with only polynomial computational effort in the input size of the problem, to an instance of this Ising partition function problem. This implies, in particular, that the existence of an efficient algorithm for this Ising partition function problem would yield an efficient algorithm for all problems in BQP.

4 References

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