A New Quantum Computing Approach to Finding the Ground State of an Ising Model

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Abstract

The Ising Spin Model is a fundamental concept in the study of Spin Glass systems, which explores particle interactions. Our research focuses on solving the Ising Model using two key algorithms: the Quantum Approximation Optimization Algorithm (QAOA) and the Continuous-time Quantum Walk (CTQW). QAOA approximates Hamiltonian minimization, allowing it to find the ground state efficiently. CTQW leverages quantum mechanics principles to explore graph structures and search for optimal solutions. By comparing and bench marking these approaches, we aim to create a novel heuristic algorithm to find a lower energy ground state using the same time complexity.

1 Background

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1.1 Ground State of the Ising Model

The Ising Spin Model is a critical component in the study of Spin Glass systems, which are concerned with the interactions of particles. In this model, each spin, denoted as σ_i , can take one of two values: +1 or -1, where σ_i represents the i-th spin. Particles with a spin quantum number of -1 have a spin orientation that is opposite to that of particles with a spin quantum number of +1 [1]. The term w_{ij} signifies the interaction between neighboring spins and their strength. It holds a value of zero for non-neighboring spins and -1 if and only if spins i and j are connected [1]. Each spin σ_i contributes its energy to the Hamiltonian of the spin system. This contribution is defined as follows [2]:

$$H(\sigma) = -\sum_{i < j} w_{ij} \sigma_i \sigma_j \tag{1}$$

This equation represents the Hamiltonian of the system, which is a measure of the total energy of the system. The ground state of the Ising model corresponds to the configuration of spins that minimizes this Hamiltonian and thus minimizes the total energy of the system. Finding the ground state of an Ising spin model can be mapped to a two-dimensional graph, where each particle can be represented as a node. Particles with spin quantum numbers of +1 and -1, which are neighbors, share an edge in the graph. Minimizing the energy of the physical system and finding it's ground state is equivalent to finding the max-cut of this graph. An example of mapping the Ising spin model to a two-dimensional graph and finding the graph's max-cut is 1.

1.2 Quantum Approximation Optimization Algorithm

The QAOA is used for many different types of optimization problems in Quantum Computing, more specifically, the QAOA can generate an approximate Hamiltonian minimization and thus in turn

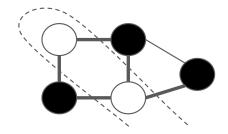


Figure 1: Example: A graph with five nodes and six edges. The dashed line represents the max-cut of this graph: the empty nodes are in set V_1 and the colored nodes are in set V_2 . There are other max-cuts, but in this graph the max-cut is five.

approximately minimize the system's energy and find the approximate ground state of the Ising Model [1]. This is represented as 1 where $\mathbf{b} \in \{0, 1\}^n$ [1].

$$C(\mathbf{b}) = \sum_{\alpha=1}^{m} C_{\alpha}(\mathbf{b}) \tag{2}$$

Equations 1 and 2 are closely related, as 1 represents the Hamiltonian that 2 is approximately minimizing. By mapping the Ising system model to the max-cut problem, we can define the QAOA by the following steps [1]:

- 1. A qubit is allocated for each node in the graph.
- 2. All qubits are initialized to a state that is an equal superposition.
- 3. By applying the $U(H_c, \gamma)$, otherwise known as the Hamiltonian cost, we are able to calculate the cut value for the given graph for an angle γ .
 - 4. By applying the $U(H_c, \beta)$, otherwise known as the Hamiltonian mixer, we are able to modify the current states of the qubits based on the cost calculated in step 3 for an angle β .
 - 5. We will repeat the previous two steps, for a total of p times with different parameters γ_i and β_i , ultimately, creating new states. p is defined as the depth chosen for the algorithm.
 - 6. Based off the function of the depth, $F_p(\gamma, \beta)$, we calculate the expected Hamiltonian cost after running the QAOA algorithm for a given depth p.

45 1.3 Random Walk

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46 1.3.1 Classical Random Walks

A particle starts out in some initial position (vertex) on a graph G = (V, E) and transitions to neighboring vertices based on a probability distribution (Policy), e.g. a pseudo-random number generator or a stochastic matrix for time evolution. At each iteration, the particle's position is updated according to a stochastic matrix [4].

$$\mathbf{p}(t+1) = M\mathbf{p}(t) \tag{3}$$

Discrete-time classical walk: Policy \mathbf{p} is updated via stochastic matrix M.

52 1.3.2 Continuous-Time Quantum Walk

By turning the Eq 4 into a differential equation we can derive Schrödinger's equation [4].

$$\frac{d\mathbf{p}(t)}{dt} = -H\mathbf{p}(t) \tag{4}$$

Excludes \hbar and i.

What makes this continuous is that the matrix H is treated as the Hamiltonian. Based on the solution $\mathbf{p}(t) = e^{Ht}\mathbf{p}(0)$ to the differential equation, the following unitary evolution is created [4].

$$U(t) = e^{iHt} (5)$$

Time evolution operator: defining a spectrum of t's 5

Motivation 58

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- Quantum computing deals with optimizing problems like Ising Model, a known NP-complete problem. 59
- Solving the Ising model enables the solution of all other NP-complete problems [3]. A solution to 60
- The Ising Model can be found by using QAOA and Random Walk algorithms in linear and sublinear 61
- time respectively, but these algorithms do not find very optimal solutions. This research aims to
- optimize solving the Ising Model on the Rensselaer Polytechnic Institute (RPI) Quantum System One,
- to understand the challenges and limitations, and develop a new alternative algorithm comparable in 64
- runtime while producing more optimal solutions than that of QAOA and Random Walk algorithms.

3 **Tentative Plan**

- 1. Implement both QAOA and Random Walk algorithms.
- 2. Execute the QAOA on a small-scale graph in Qiskit SDK v1.1 using the RPI IBM Quantum System One and benchmark its performance.
- 3. Execute the Random Walk on the same small-scale graph in Qiskit SDK v1.1 using RPI 70 IBM System One and benchmark its performance.
 - 4. Design a new alternative heuristic algorithm to solve the Ising problem.
 - 5. Implement the developed algorithm designed in Oiskit SDK v1.1 using RPI IBM Quantum System One, aiming to surpass the bench marked results.

Expected Results and Take Home Message 75

- Using the benchmarks of QAOA and Quantum Walk, develop a new heuristic algorithm that finds 76
- the ground state of an Ising system. By performing a comparative analysis, we will attempt to beat 77
- the results of the benchmarked algorithms and understand the specific strengths and weakness in our 78
- algorithm and areas for potential future improvement.

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