Disordered Phase in Ising and Metastability in Cellular Potts Models Hint at Glassy Dynamics

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Abstract

In this paper, quantum algorithms are to be used to simulate glassy systems in toy models. To look for glassy behaviour, the energy landscape and spin configurations of the transverse field Ising model in a longitudinal field are studied. The Variational Quantum Eigensolver (VQE) is used to obtain the ground-state energies and corresponding eigenstates for a 6×6 Ising lattice using 36 qubits and a 1-dimensional Ising chain of length 25. For the 8×8 Cellular Potts model, the original Hamiltonian is converted to an Ising formulation for the VQE to reduce to its ground state. The energy change during minimization is carefully analysed to find whether the effects of interfacial tension among cells could probably induce glassiness in the cell system.

1 Introduction

Glassy dynamics have been emergent in disordered quantum mechanical systems. The transverse Ising model in a longitudinal field [1][2] exhibits disordered spin systems [3][4] that are pivotal in studying complex systems and related investigations. The glassiness in these models are systems with quenched spin disorder and relaxed spin-flip dynamics. The disordered phase in these models can help model many near-optimal solutions to combinatorial optimization problems, neural networks, minority games, etc.[5][6]. These solutions refer to the local minima in the energy landscape, thereby indicating metastability in its phases. Biological cells in dense tissue exhibit many glassy properties and are found in diverse biological processes like wound healing, embryonic development, and cancer metastasis. The Cellular Potts model is used to study the glassy nature of these cells[7]. In this paper, we aim to study these models using a quantum computer.

2 Methodology

In order to simulate glassy dynamics on a quantum computer, we have primarily studied two models: The Ising model and the Cellular Potts model. The grounds state energies of the models were found out using Variational Quantum Eigensolver algorithm.

2.1 The Transverse Ising Model In A Longitudinal Field

The Hamiltonian of the model is written in tensor products of Pauli operators and is given by[3]: $\mathcal{H} = J \sum_i \sigma_i^z \sigma_{i+1}^z - B_x \sum_i \sigma_i^x - B_z \sum_i \sigma_i^z$. Here, B_x represents the transverse Field and B_z represents the longitudinal field, the Pauli Z operators representing the spins and the Pauli X operator representing the Transverse field. J is the interaction term. The Transverse field induces quantum fluctuations.

2.1.1 The 1-Dimensional Simulation

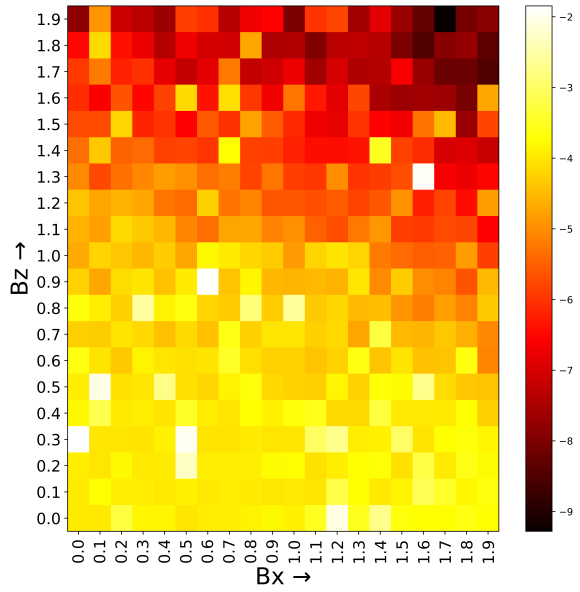
For the 1-Dimensional case, we have considered a 1D Ising Model of chain length 25. The Hamiltonian $\mathcal{H}$ is so constructed using a custom-coded utility that prints out the Hamiltonian using elementary Pauli operators[2]. This 25 qubit Hamiltonian is then fed into a Variational Quantum Eigensolver algorithm, that used a TwoLocal ansatz. The ansatz uses R_x and R_y rotation blocks with no entanglement in them. The VQE uses a `COBYLA` optimizer whose maximum iterations are set at 25,000 iterations. The `Qiskit Aer_gpu` backend to simulate the VQE algorithm.

2.1.2 The 2-Dimensional Simulation

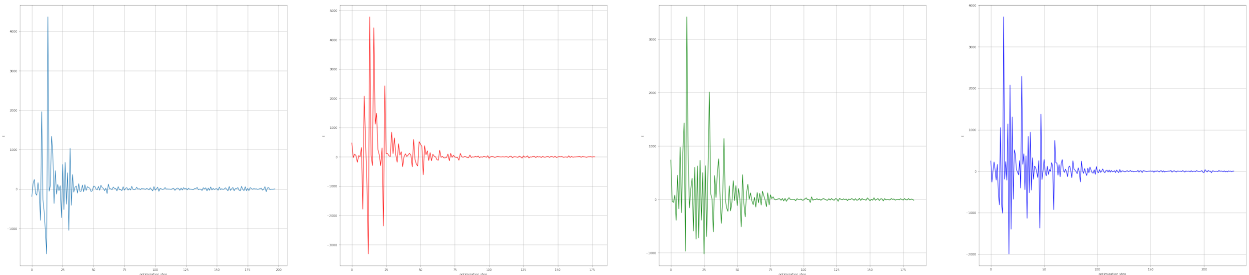
When considering the 2-Dimensional case, the Ising model was constructed on a square lattice of 6×6. The Hamiltonian $\mathcal{H}$ is so constructed using a custom-coded utility that prints out the Hamiltonian using elementary Pauli operators. This 36 qubit Hamiltonian is then fed into a Variational Quantum Eigensolver algorithm, that uses a TwoLocal ansatz. The ansatz uses R_x and R_y rotation blocks with no entanglement in them. The VQE used a `COBYLA` optimizer whose maximum iterations were set at 25,000 iterations. We used the `matrix_product_state` method on the `AerSimulator` backend to simulate the VQE algorithm.

2.2 The Cellular Potts Model

This section outlines the methodology to simulate glassy dynamics in biological tissue with 7 different types of biological cells with preserved continuity, placed along an 8×8 lattice. The cells in this model are evolved by updating all the lattice sites in the cell by using a Variational Quantum Eigensolver acting on an Ising formulation of the Hamiltonian [8] $\mathcal{H}$, given by: $\mathcal{H} = \mathcal{H}_{\mathcal{A}} + \mathcal{H}_{\mathcal{B}} + \mathcal{H}_{\mathcal{J}} = \sum_i^N \{\lambda_A (A_i - A_0)^2 + \lambda_P (P_i - P_0)^2\} + \sum_{\langle ij \rangle} J(\sigma_i, \sigma_j)$, where $J(\sigma_i, \sigma_j) = 0$ when $\sigma_i = \sigma_j$ and $J(\sigma_i, \sigma_j) = \alpha$ when $\sigma_i \neq \sigma_j$. Here, $\langle i, j \rangle$ denotes the von Neumann nearest neighbour, A_i and P_i are the areas and perimeters



(a) Energy Landscape for 1D Ising model for varying B_x and B_z



(b) Plots for $J = 1$ (c) Plots for $J = 2$ (d) Plots for $J = 3$ (e) Plots for $J = 4$

Figure 1: Plots of the results of the 1-dimensional Ising Model (a). The first order derivatives denoting the energy fluctuations while minimizing the Cellular Potts model to its ground state using VQE for increase in J are shown in plots (b)-(e)

of the i^{th} cell. A_0 and P_0 are the target and perimeter of the cells. λ_A and λ_P are the elastic constants associated with area and the perimeter respectively. Intercellular repulsion between two cells σ_i and σ_j is given by the parameter J, chosen to be same for all cells.

The Hamiltonian $\mathcal{H}$ translates to a quadratic minimization problem for IBM `docplex` and subsequent conversion to an Ising Hamiltonian. This Hamiltonian is then subject to a VQE that uses the TwoLocal ansatz on eight qubits, with no entanglement on R_y and R_z rotation blocks, paired with 500 iterations of the `COBYLA` optimizer.

3 Observation and Discussion

3.1 Transverse Ising Model in a Longitudinal Field

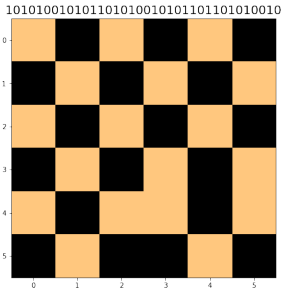
3.1.1 1D simulation

We observe in the energy landscape thus generated (Figure 1(a)), that an increase in the longitudinal field leads to a lower energy of the Hamiltonian, but an increase of the transverse field does not lower the energy as much. The role of the transverse field is primarily to induce quantum effects[2][9]. These quantum effects give a rise to alternating ferromagnetic and anti-ferromagnetic interactions, which in turn produces the disordered phase.

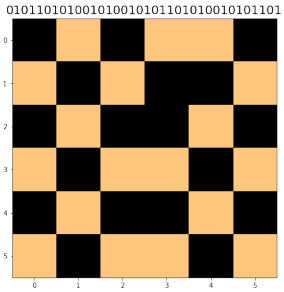
3.1.2 2D simulation

Here, the most notable thing to see is that the best three configurations for each case are near identical: a pattern arises in simulations, indicating that a coherent study is possible. We can now see the disordered phase region, which most published literature does not account for [10]. The spin configurations with the highest counts/probabilities of occurrence are shown in Figure 2. All the configurations along with their counts have been provided as a supplement in the project repository.

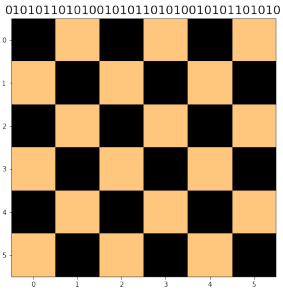
When $B_z = 0$ and $B_x = 2$, we can see a perfect anti-ferromagnetic spin configuration in the absence of the longitudinal field. The configuration with the 2^{nd} and 3^{rd} highest counts shows near-perfect anti-ferromagnetism as well. We hypothesize that a longitudinal field is essential for a disorder



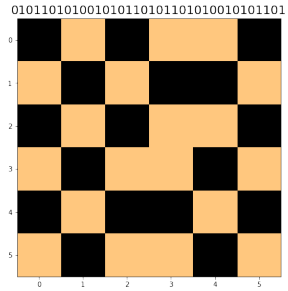
(a) $B_z = 1, B_x = 0.5$



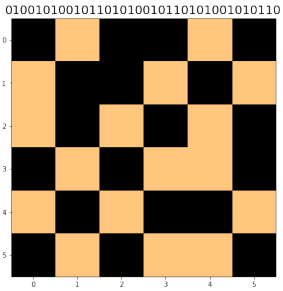
(b) $B_z = 1.5, B_x = 0.25$



(c) $B_z = 0, B_x = 2.0$



(d) $B_z = 1, B_x = 2.0$



(e) $B_z = 1.5, B_x = 1.5$

Figure 2: The plots for the 2D Ising model with $J = 1$ and varying B_x and B_z

to occur. This is seen in the spin configurations when $B_z = 1$ and $B_x = 2$, where we see a mixture of anti-ferromagnetic and ferromagnetic spin configurations, i.e., a disordered state. The ferromagnetism is seen in local moments.

If we compare cases $B_z = 1$, $B_x = 0.5$ with $B_z = 1$, $B_x = 2$, we see that for the same values of B_z, an increase in disorder occurs with the increasing B_x. $B_z = 1, B_x = 0.5$, shows mostly anti-ferromagnetism, whereas $B_z = 1, B_x = 2$, develops local moments of ferromagnetism. $B_z = 1.5, B_x = 1.5$ shows a relatively more paramagnetic state i.e., spins are more random. Further increase of B_z, in theory, should increase the randomness. Decreasing B_x , $B_z = 1.5$, $B_x = 0.25$, shows a disordered state. Therefore, we observe a disordered state only for a specific combination of values of the transverse and longitudinal Ising fields i.e., the disordered phases occupy a narrow region between the anti-ferromagnetic phase and the paramagnetic phase [11].

3.2 Cellular Potts Model

We observe in Figure 1 (b)-(e) that as the values of the interfacial tension (J) increases from $J = 1$ to $J = 4$, the fluctuation of the total energy of the system, as it is being minimized by the VQE, increases. This implies that for lower values of J, the VQE was able to minimize the energy of the system with comparatively lower number of local minima or metastable states. This is because the interfacial tension between the cells resists the minimization of the energy to it's ground state as theorized by [12] [13] [14].

4 PROPOSED QISKIT MODULE

We are in the process of constructing a dynamic, modular package `QuGlassyIsing` for glassy dynamics that interfaces with Qiskit. The package employs custom-built functions for easily constructing the Hamiltonians, which can then be used to feed into a VQE to arrive at a ground state. As of writing this article, `QuGlassyIsing` has a release candidate `v0.0.1-alpha`.

5 CONCLUSION AND FUTURE SCOPE

In this paper, we have shown, that by simulating small scale, toy models using quantum computers, we were able to detect disordered phases in 1D and 2D Ising models thereby, hinting at the formation of glass therein. We have observed the importance of the longitudinal field in the Ising models for developing regions of disorder, between states of anti-ferromagnetic and ferromagnetic states. We have also seen hints of glass formation in biological tissues using Cellular Potts models by observing the increased metastability for increasing values of interfacial tension coefficients. This research paves the way for the study of the glassy behaviour of systems using quantum computers in the NISQ era. We hope to utilise the full potential of quantum computers in the post-NISQ era to simulate glassy behaviour more concretely.

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