Applying Adiabatic Quantum Computing to Optimisation Problems

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The maximum independent set (MIS) problem is a classical NP-hard optimisation challenge with applications ranging from graph colouring to protein structure design. In this research, we apply Adiabatic Quantum Computing (AQC) to approximate solutions for a 5-qubit instance of the MIS problem, encoded into an Ising model Hamiltonian. Using Python-based simulations, the quantum state is evolved from an initial superposition to the MIS solution. In this research, we investigate the algorithm's behaviour and success probabilities across varying runtimes, revealing the requirements for adiabatic evolution.

1. Encoding Optimisation Problems

Many classical optimisation problems are **NP-hard**, meaning they are computationally difficult to solve efficiently. Examples include scheduling and stock portfolio optimisation. Quantum computing offers new approaches, as quantum algorithms have shown the potential to outperform classical methods of solving such problems. This is an active area of research, with notable examples such as Shor's algorithm for factorising large integers, demonstrating strong evidence of exponential speedup [1].

In this research, we explore quantum optimisation for solving the **Maximum Independent Set (MIS)** problem. This problem involves identifying the largest subset of vertices (nodes) in a graph such that no two vertices in the subset are directly connected by an edge (line). One approach is to encode the MIS problem into a quantum system by using the **Ising model**, represented by the Hamiltonian

$$H_{Ising} = \sum_{k=1}^{n} \sum_{j=k+1}^{n} J_{kj} \sigma_k^z \sigma_j^z + \sum_{j=1}^{n} h_j \sigma_j^z , \tag{1}$$

where the coefficients J_{kj} form an adjacency matrix M encoding the graph's connectivity and the terms h_j penalise configurations that do not satisfy the MIS. The penalties are enforced within the vector given by

$$h_j = -\left(\sum_j M_{kj} + M_{jk}\right) + \kappa, \tag{2}$$

where setting $\kappa = 1/2$ ensures higher energies are assigned to invalid configurations; thus, the ground state of H_{Ising} encodes the MIS solution for a given graph.

The Pauli-Z operator σ_j^z is applied to the jth qubit, leaving all other qubits unchanged with the expression

$$\sigma_j^z = \left(\otimes_{k=1}^{j-1} I_2\right) \otimes \sigma^z \otimes \left(\otimes_{k=j+1}^{n} I_2\right), \tag{3}$$

where I_2 is the identity matrix. An example of a graph G with 5 qubits is displayed in Fig. (1), used in this research.

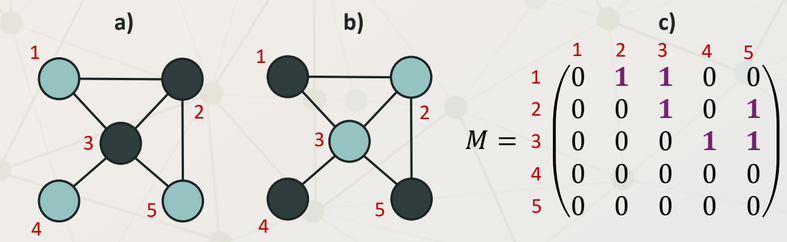

Fig. (1): A graph with some vertices coloured in dark green. a) A configuration which does not form an MIS. b) The MIS solution for this graph. c) Adjacency matrix encoding the graph; 1s located where the two labelled nodes are connected, 0 otherwise

2. Adiabatic Quantum Computing

The approach used in this work to solve quantum optimisation problems is known as **Adiabatic Quantum Computing (AQC).** This paradigm is based on the adiabatic theorem, which states that a quantum system will remain in the instantaneous ground state of a time-dependent Hamiltonian $H(t)$ as this operator evolves, provided that $H(t)$ evolves sufficiency slowly [2]. This evolution is governed by the **transverse field Ising model**

$$H(t) = -A(t) \sum_j \sigma_j^x + B(t) H_{Ising}, \tag{4}$$

where $A(t)$ and $B(t)$ are **annealing schedules** that control the relative strengths of the transverse field term (encoded by the Pauli-X operator σ_j^x) and the problem-specific Ising Hamiltonian [3]. They are defined as linear functions of time,

$$A(t) = 1 - \frac{t}{t_{max}} \quad \text{and} \quad B(t) = \frac{t}{t_{max}}, \tag{5}$$

where t_{max} is the total runtime of the algorithm. At $t = 0$, the system is prepared in the ground state $\psi_g = |\psi(t=0)\rangle$ corresponding to a linear superposition of all possible configurations.

3. Adiabaticity and Timescales

To ensure the system remains in the ground state throughout the evolution $t \in [0, t_{max}]$, the **fidelity** $\mathcal{F}$, defined as

$$\mathcal{F} = \left|\langle \psi_g | \psi(t = t_{max}) \rangle\right|^2, \tag{6}$$

must remain as close to 1 as possible. $\mathcal{F} \approx 1$ signifies that the final state corresponds to the ground state of H_{Ising}.

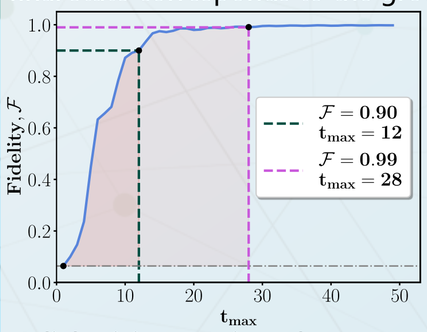

Fig. (2): Final fidelity as a function of t_{max} for the graph G. Key thresholds at $\mathcal{F} = 0.90$ and $\mathcal{F} = 0.99$ are marked, with the corresponding t_{max} values. Beyond $t_{max} = 28$, the fidelity approaches 1, suggesting successful adiabatic evolution and convergence to the MIS solution.

Adiabaticity requires that $H(t)$ evolves slowly, which is driven by t_{max}. This depends on the **minimum energy gap** g_{min} between the ground and first excited state energies, and the Hamiltonian rate of change ε [4]:

$$t_{max} \gg \frac{\varepsilon}{g_{min}^2}. \tag{7}$$

Here, the evolution timescale is set by g_{min}, as smaller gaps require longer runtimes to prevent non-adiabatic jumps.
In this work, a sufficiently high level of adiabaticity is achieved at $t_{max} = 28$, as seen in Fig. (2).

4. Simulation Results

Simulating the adiabatic algorithm requires the use of an **evolution operator** U, defined analytically as

$$U(t_{max}, 0) = \lim_{q \to \infty} \tau \prod_{j=1}^{q} \exp\left\{-i \frac{t_{max}}{q} H\left(\frac{j t_{max}}{q}\right)\right\}, \tag{8}$$

where τ indicates time-ordering. This is approximated numerically by choosing a finite number of time-steps q. Thus, the system evolves through repeated iterations of U to give the new state at a time $\frac{k t_{max}}{q}$, setting k as the iteration index.

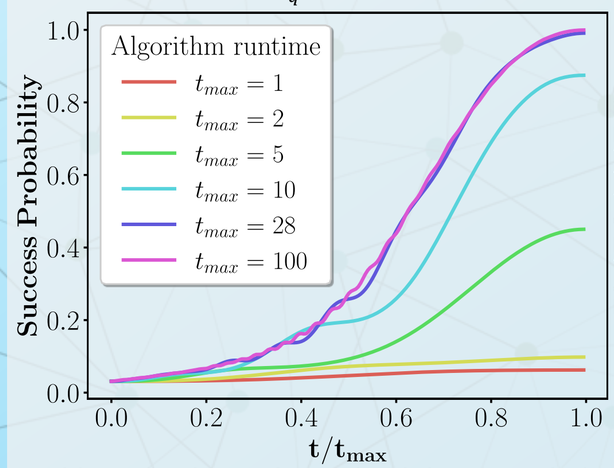

Fig. (3): The instantaneous success probability as a function of t/t_{max} for the graph G, scaled for six different values of t_{max}. The probability of finding the MIS solution approaches 1 for larger t_{max}.

In this research, we determined the MIS solution to the graph G and simulated the algorithm in Python for various t_{max} values, choosing $q = 200$. At each iteration, the success probability P of finding the MIS solution is calculated using the **Born rule**

$$P = \left|\langle \psi_f | \psi(t) \rangle\right|^2, \tag{9}$$

where $|\psi_f\rangle$ is the target MIS solution state. Fig. (3) shows the results; for $t_{max} > 28$, the probability of finding the MIS solution approaches 1, consistent with adiabatic evolution.

References

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