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Towards Optimal Graph Coloring Using Rydberg Atoms

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Quantum mechanics is expected to revolutionize the computing landscape in the near future. Among the many candidate technologies for building universal quantum computers, Rydberg atoms-based systems stand out for being capable of performing both quantum simulations and working as gate-based universal quantum computers while operating at room temperature through an optical system. Moreover, they can potentially scale up to hundreds of quantum bits (qubits). In this work, we solve a Graph Coloring problem by iteratively computing the solutions of Maximal Independent Set (MIS) problems, exploiting the Rydberg blockade phenomenon. Experimental results using a simulation framework on the CINECA Marconi-100 supercomputer demonstrate the validity of the proposed approach.

CCS Concepts: • **Hardware → Quantum computation**.

Additional Key Words and Phrases: quantum computing, neutral atoms, graph coloring, optimisation

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1 INTRODUCTION

Quantum Computing is projected to be the next step in the evolutionary path of the computing domain. At its basis lie the laws of quantum mechanics that provide the building blocks for defining computing systems theoretically able to outperform any other classical (super)computer in specific application fields, e.g., combinatorial optimization problems. Among the many technologies that can be used to implement such systems, optical ones manipulating Rydberg atoms have been recently found to be promising. Indeed, contrary to many competitors, this technology operates at room temperature and it is flexible enough to create quantum gates as well as manipulating a given target system Hamiltonian. In this work, we explored this latter feature to solve the Graph Coloring problem (GC). Specifically, the proposed quantum-based heuristic solves the GC problem by iteratively solving a Maximal Independent Set (MIS) problem. To this end, a register of Rydberg atoms is constructed in such a way it directly maps on the graph structure of the problem. The proposed heuristic was demonstrated to be effective in using a number of colors that is close to the optimal solution. As such, it can represent a step towards solving large instances of industrial optimization problems such as the Physical Cell Identifier Assignment problem in cellular networks.

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2 SOLVING THE GRAPH COLORING PROBLEM WITH ITERATIVE MIS

Atoms can be excited from ground to a specific quantum state referred to as the Rydberg state by applying a specific sequence of laser pulses. Atoms in this state can interact with each other; however, the effect of their mutual interaction strongly decays with the increasing of their relative distance (i.e., the strength of the interaction is proportional to $|r_i - r_j|^{-6}$) as reported by the Hamiltonian describing the system [1]:

$$\mathcal{H} = \sum_{i=1}^{N} \frac{\hbar\Omega}{2}\sigma_i^x - \sum_{i=1}^{N} \frac{\hbar\delta}{2}\sigma_i^z + \sum_{j<i} \frac{C_6}{|r_i - r_j|^6} n_i n_j$$

where Ω and δ are respectively the Rabi and detuning frequencies of the controlling laser system. Interestingly, if the relative distance between excited atoms is less than the Rydberg blockade radius (i.e., $r_b = (\frac{C_6}{\hbar\Omega})^{1/6}$), they are prevented to be in the Rydberg state at the same time. Given that, by arranging the Rydberg atoms' position in such a way that it maps the input graph structure, then the Rydberg blockade phenomenon allows to directly obtain a set of candidates MIS solutions with a limited computing cost by using a Quantum Approximate Optimization Algorithm (QAOA) approach [1]. Indeed, Rydberg atoms within the r_b radius represent graph nodes sharing an edge, with the whole register laid out as a *Unit Disk graph* (UD). The GC problem can be solved by iteratively selecting one MIS of the graph: at each iteration, a new set of MIS solutions is generated, and the most promising one is chosen (i.e., it corresponds to assign a new color to the graph), then a sub-graph is derived by removing the nodes belonging to the MIS (Greedy-itMIS). A further improvement is given by hybridizing this procedure with a Branch and Bound (BB) strategy: a BB tree is constructed, based on the fact that alternative solutions for the MIS are generated (i.e., the measurement of the final state of the quantum system –Rydberg atoms' register– results in a distribution of feasible solutions), then it is explored to choose the optimal set of MIS solutions (BB-itMIS). Moreover, the exploration of the BB tree can be parallelised.

Vertices	Greedy-itMIS	BB-itMIS	Optimum
10	3 colors	3 colors	3 colors
11	3 colors	3 colors	3 colors
12	4 colors	3 colors	3 colors
13	4 colors	3 colors	3 colors
14	4 colors	3 colors	3 colors
15	4 colors	3 colors	3 colors
16	4 colors	3 colors	3 colors
17	4 colors	3 colors	3 colors

Table 1. Comparison between the optimal graph coloring and the iterative MIS-based approaches using the Pulser library.

Vertices	Greedy itMIS	BB-itMIS	Optimum
25	4 colors	3 colors	3 colors
35	5 colors	5 colors	5 colors
45	8 colors	6 colors	6 colors
55	7 colors	7 colors	7 colors
65	8 colors	8 colors	7 colors
75	10 colors	9 colors	8 colors
85	10 colors	9 colors	8 colors
95	11 colors	9 colors	8 colors

Table 2. Validation of the approach using state-of-the-art QUBO solver.

The first set of results (Table 1) is obtained with a simulation framework [2] that models the physics of the Rydberg atoms, hence fully reflecting the behaviour of the upcoming machine. To validate the itMIS approach for larger graphs, due to the high cost of the full simulation, we also performed experiments replacing the MIS solver with a numerical one while keeping the same global approach (Table 2). Experiments are performed on Cineca MARCONI100. Both sets of results are extremely satisfactory in terms of the number of colors used vs. the exact solution: we expect that this methodology scales well with the number of qubits on a physical machine, providing an efficient approach to solve graph coloring problems on neutral atoms quantum computers.

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