Rydberg quantum wires for maximum independent set problems

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One application of near-term quantum computing devices is to solve combinatorial optimization problems such as non-deterministic polynomial-time hard problems. Here we present an experimental protocol with Rydberg atoms to determine the maximum independent set of graphs, defined as an independent set of vertices of maximal size. Our proposal is based on a Rydberg quantum wire scheme, which exploits auxiliary atoms to engineer long-ranged networks of qubits. We experimentally test the protocol on three-dimensional Rydberg atom arrays, overcoming the intrinsic limitations of two-dimensional arrays for tackling combinatorial problems and encode high-degree vertices. We find the maximum independent set solutions with our programmable quantum-wired Rydberg simulator for Kuratowski subgraphs and a six-degree graph, which are paradigmatic examples of non-planar and high-degree graphs, respectively. Our protocol provides a way to engineer the complex connections of high-degree graphs through many-body entanglement, taking a step towards the demonstration of quantum advantage in combinatorial optimization.

Quantum information and quantum computing have drawn significant interest in recent years because of their potential for solving computational problems which are intractable for non-quantum computational methods. These quantum approaches could be beneficial, in particular, for computational problems that are hard to classical devices but relatively easy to quantum devices. Combinatorial optimization problems aim to find an optimal solution from feasible solutions. One example is the maximum independent set (MIS) problem in graph theory, which seeks to find an independent vertex set of maximal size for a graph, as explained in more detail below. While the MIS problem is classical by definition, its computational complexity (NP complete) makes it intractable to classical Turing machines. Alternatively, if a quantum many-body system allows an intrinsic mapping of the problem to, for example, the many-body ground state, its evolution might be engineerable for the benefit of computational speed-up.

Rydberg atom systems provide an intrinsic Hamiltonian for the MIS problem of particular relevance in the context of the present paper. Let us consider N atoms arranged into a graph \( G = (V, E) \), where \( V \) and \( E \) represent the individual atoms and Rydberg-blockaded atom pairs, respectively. The Hamiltonian is approximately given by

\[
H_G = U \sum_{(j,k) \in E} \hat{n}_j \hat{n}_k - \frac{\hbar \Delta}{2} \sum_{j \in V} \hat{\sigma}^z_j,
\]

where \( U \) is the nearest-neighbour interaction, \( \Delta \) is the laser detuning and \( \hat{n} = (\hat{n}^2 + 1)/2 \) is the Rydberg excitation. The configuration \( n = 1 \) (\( n = 0 \)) is for the Rydberg (ground) state of each atom. The first term prohibits adjacent Rydberg atoms from making an independent set of \( G \), while the second term, for \( \Delta > 0 \), favours maximal Rydberg atoms. So, the many-body ground state of \( H_G \) gives the independent vertex set of maximal size, that is, the MIS solution \( M(G) \) of \( G \) (refs. 1,19), with anti-ferromagnetic strong coupling (\( U > \hbar \Delta \)) and a positive detuning field (\( \Delta > 0 \)). For example, a two-dimensional (2D) Rydberg atom array is presented in Fig. 1a with a four-vertex graph \( G \) being the 3-pan graph in the nomenclature of the Information System on Graph Classes and their Inclusion (https://www.graphclasses.org). The atom arrangement, illustrated by the numbering in Fig. 1a, is suitable to utilize the Rydberg blockade with a radius, \( r_n \) and its ground state \( \{|00\rangle + |11\rangle\}/\sqrt{2} \) gives two independent sets, that is, the MIS solution \( M(3\text{-}pan) = \{|1,3\}, \{|1,4\}\} \) of \( G \), by counting the \( |n = 1\) atoms. Thus, quantum simulations for the ground state of the Schrödinger equation, \( \hat{H}_G \) \( M(G) \) = \( E(G) \) \( M(G) \), find the MIS solutions.

We note two intrinsic limitations of two-dimensional (2D) Rydberg atom arrays for MIS problems. First, non-planar graphs...
Fig. 2 | Experimental tests of Rydberg quantum wires. a–c, A test graph set, \(G_0 = P_4, G_1 = C_4, G_{2+ w} = C_6\), for the algorithm with no frustration, that is, \(\hat{M}(G_T) = \hat{M}(G_{0+ w})\), where \(G_0 = P_4, G_1 = C_4, G_{2+ w} = C_6\), in which atoms 1–4 are qubits and atoms 5 and 6 form the quantum wire. d–f, Experimental probability distributions, indicating the MIS solutions (grey bars), the atoms in – – – dashed (l), the ground state of the Hamiltonian is obtained by solving the \(\hat{H}_{G_{0+ w}}\), where \(G_0 = P_4, G_1 = C_4, G_{2+ w} = C_6\), in which atoms 1–4 are qubits and atoms 5 and 6 form the quantum wire. g–i, A test graph set, \(G_2 = G_4, G_3 = 3-\text{pan}, G_{4+ w} = 5-\text{pan}\), for the algorithm with frustration, that is, \(\hat{M}(G_T) = \hat{M}(G_{0+ w}) - \hat{F}(G_{0+ w})\), where \(G_0 = C_4, G_1 = 3-\text{pan}, G_{2+ w} = 5-\text{pan}\), in which atoms 1–4 are qubits and atoms 5 and 6 form the quantum wire. The experimental probability distribution of \(S_4\) showing \(\hat{M}(S_4) = \{(2, 4), (1, 4), \hat{F}(G_{0+ w}) \}\) (blue bars), to couple the qubit atoms A and B. If the quantum wire is treated as an edge, the combined graph \(G_{2+ w}\) is equivalent to the target graph, \(G_6\), that is the Moser spindle graph. Whether the quantum wire is implemented as such can be post-selected by investigating the frustration of the atoms A and B among the MIS solution \(\hat{M}(G_{0+ w})\).

The second operation, \(\hat{F}\), is to project quantum states in the enlarged Hilbert space of \(G_{2+ w}\) onto the Hilbert space of the target graph \(G_6\), which can be done readily by measuring the qubit information of \(G_T\). Hereafter, we introduce the bar notation to specify the projection, for example, \(\hat{M}(G) \rightarrow \hat{M}(G)\). The second operation, \(\hat{F}\), is to remove configurations with frustration between qubits at the boundaries, the atoms A and B in Fig. 1b, when some elements \(\hat{F}(G_{0+ w})\) of \(\hat{M}(G_{0+ w})\) violate the Rydberg blockade condition. Then, the MIS solution of \(G_T\) is obtained as

\[
\hat{M}(G_T) = \hat{M}(G_{0+ w}) - \hat{F}(G_{0+ w})
\]
(see Methods for detailed discussions). Note that our Rydberg quantum wire scheme utilizes quantum entanglement of the two quantum many-body systems, that is, the original graph and the wire. Namely, qubits of the two systems become entangled so that the MIS solution of a target graph is accessible.

Quantum simulation of MIS problems is performed with quantum annealing of three-dimensional (3D) atom arrays\(^3\). In experiments, neutral \(^{87}\)Rb atoms are arranged in free space in such a way that all the nearest-neighbour atom pairs, which describe the edges of the graphs, are kept at a fixed interatomic distance \(d\) that is smaller than the Rydberg blockade radius, that is, \(d < r_b = (2\hbar/\Omega)^{1/6} = 9.8 \mu\text{m}\), and that all other atom pairs, which are not connected by edges, are at distances longer than \(\sqrt{2}d > r_b\) (refs. \(^2\,\^3\)). The ground state \(|SS_{L2}, F = 2, m_F = 2\rangle = |n = 0\rangle\) and the Rydberg state \(|715_{L2}, m_I = 1/2\rangle = |n = 1\rangle\) of each atom are used for the qubit two-state system. An effective Hamiltonian of the 3D atom arrays is

\[
\hat{H}(t) = U \sum_{(jk) \in E} \hat{n}_j \hat{n}_k - \frac{\hbar}{2} \sum_{j \in V} \left( \delta(t) \hat{\sigma}_j^z - \Omega(t) \hat{\sigma}_j^y \right),
\]

where the Pauli matrices with the two states at sites \(j\) and \(k\) are introduced with \(\hat{\sigma}_j^z = (\hat{\sigma}_j^x + 1)/2\). The terms on the right-hand side describe the van der Waals interaction at the fixed distance \(d\), the time-dependent detuning and the time-dependent Rabi frequency, respectively. Initially, the atoms are prepared with paramagnetic down spins at \(t = 0\), \(|00 \cdots 0\rangle\), with \(\delta(0) = \Delta_c < 0\) and \(\Omega(0) = 0\). To find the MIS solutions of \(G\), these atoms are quasi-adiabatically driven to the many-body ground state \(|H_G\rangle\), by turning on and off the Rabi frequency while the detuning is gradually increased to \(\delta(t = t_f) = \Delta_c < U\) (ref. \(^2\)) (see Supplementary Information and refs. \(^2\,\^3\,\^4\) for details).

We first consider in Fig. 2 experimental tests of Rydberg quantum wires for the cases with and without frustration, that is, \(\tilde{F}(G_{0+w})\) being \(\emptyset\) or not in equation (3), respectively. For graphs without frustration, we consider the initial graph, \(G_0 = P_5\) (the four-vertex path graph) in Fig. 2a, and the target graph, \(G_t = C_4\) in Fig. 2b. The construction of the wired graph, \(G_{0+w} = C_4\) is done by adding an \(M = 2\) Rydberg quantum wire (red spheres) as shown in Fig. 2c. Quantum simulations observe high-population states as in Fig. 2d–f, whose MIS solutions are summarized as \(M(G_{0+w}) = \{\{2, 4\}, \{1, 4\}, \{1, 3\}\}\) and \(M(G_t) = \{\{2, 4\}, \{1, 3\}\}\). It is easy to verify that \(\tilde{F}(G_{0+w}) = \emptyset\) and \(\tilde{F}(G_t) = \emptyset\), satisfying the MIS solution in equation (3). Note that the population difference among the MIS solutions of \(G_0\) (Fig. 2d) is due to the fact that the quantum annealing results in a coherent superposition of the MIS solutions, \(\tilde{M}(G_{0}) = (|0101\rangle + |1010\rangle)/\sqrt{2} + |1001\rangle/2\).

For graphs with frustration, that is, \(\tilde{F}(G_{0+w}) \neq \emptyset\), we consider the initial and target graphs, \(G_0 = S_5\) and \(G_t = 3\text{-pan}\) as in Fig. 2g,h. The wired graph is \(G_{0+w} = 5\text{-pan}\), constructed with the Rydberg quantum wire as shown in Fig. 2i. Quantum simulations of \(G_0, G_t\) and \(G_{0+w}\) are shown respectively in Fig. 2j,k,l, where the high-population states are given by \(\tilde{M}(G_0) = \{\{1, 2, 4\}\}\), \(\tilde{M}(G_t) = \{\{1, 4\}\}\), \(\{\{1, 4\}\}, \{2, 4\}\) and \(\tilde{M}(G_{0+w}) = \{\{1, 4\}\}, \{2, 4\}\). The results also confirm the MIS solutions, \(\tilde{M}(G_t) = \tilde{M}(G_{0+w}) - \tilde{F}(G_{0+w})\), where \(\tilde{F}(G_{0+w}) = \{\{1, 2, 4\}\}\) is the frustrated configuration.

Next, we consider non-planar graphs, focusing on Kuratowski subgraphs, \(K_5\) and \(K_{3,3}\). The seminal work by Kuratowski showed that a graph \(G\) is non-planar if and only if \(G\) contains any of these two Kuratowski subgraphs\(^5\). \(K_5\) in Fig. 3a is a complete graph with each vertex edged to all other vertices, and \(K_{3,3}\) in Fig. 3b is a bipartite graph with three vertices on one side completely connected to the vertices on the other side. It has been shown that both of these graphs require 3D atom arrangements\(^6\,\^7\) as well as quantum wiring.
As an additional application of Rydberg quantum wires, we consider a graph with a high-degree vertex (Fig. 4). Implementation of a high-degree vertex is crucial in quantum simulations with Rydberg atom arrays. For example, the star graph $S_6$ in Fig. 4a, which has a six-degree vertex at the centre, cannot be simulated in any 2D arrays without a quantum wire scheme, because a naive 2D implementation of atoms results in a different graph, the wheel graph $W_5$, as shown in Fig. 4b. Our strategy is to reduce the degree of the high-degree vertex using a tree-like structure of quantum wires, also known as vertex-splitting in graph theory\(^\text{32}\) and minor-embedding in adiabatic quantum computation\(^\text{11}\). As shown in Fig. 4c, the 13-vertex extended tree-like graph (red and blue spheres), $S_{6}^{\text{exp}}$, is constructed from the initial graph, $7K_3$, of seven isolated vertices. Three quantum wires are used to split the six-degree centre vertex by adding the three three-degree vertices. Quantum annealing results of the as-constructed $S_{6}^{\text{exp}}$ are shown in Fig. 4d. A single peak is observed, corresponding to the MIS solution of $S_{6}^{\text{exp}}$, which is not frustrated ($\vec{F}(G_{\text{split}}) = \emptyset$), that is, $\mathcal{M}(S_6) = \{\{2, 3, \ldots, 7\}\}$. And the Rydberg quantum wire scheme successfully constructs the high-degree graph. Note that there are no limits to the maximum degree of a vertex, as a hierarchical tree-like structure of quantum wires allows infinite degree of a vertex.

In summary, we have experimentally demonstrated the Rydberg quantum wire scheme, which utilizes Rydberg many-body interactions along a chain of neutral atoms to programme the complex connections of non-planar and high-degree graphs necessary for general MIS problems. We have used 3D arrays of qubit and quantum-wire atoms, to construct the Kuratowski subgraphs, $K_3$ and $K_{1,3}$, and the six-degree graph, $S_6$, and probed their many-body ground states using the near-adiabatic quantum annealing procedure. The observed ground states of the quantum-wired systems exhibited excellent agreement with, or algorithmically retrieved, the MIS solutions of the target graphs. Our demonstration suggests that a general graph of $N \times N$ couplings is, in principle, implementable by using Rydberg quantum wires, while there remain unresolved issues such as limited physical resources\(^\text{1}\), efficient many-body ground-state probing\(^\text{18}\) and technical issues related to tangled 3D wires. It is hoped that this quantum wire scheme demonstrated for MIS problems shall be useful to further developments for other optimization problems.

Online content
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**Methods**

**Quantum mechanics of wired MIS problems.** Our goal is to find the MIS solutions of a target graph, $G_T$, which can be obtained by finding the ground states of the Schrödinger equation of the target Hamiltonian

$$\hat{H}_T \ket{M(G_T)} = E_T \ket{M(G_T)} .$$

However, the construction of $G_T$ is fundamentally limited by non-planar graphs and high-degree vertices.

Our strategy to overcome these limitations is to investigate a wired graph, $G_{w+}$, and obtain the MIS solutions of $G_{w+}$. The basic fact is the relation, $M(G_T) \subset M(G_{w+})$, which can be easily shown by replacing an edge of $G_T$ by a quantum wire. The MIS solutions of $G_{w+}$ are obtained by solving the Schrödinger equation

$$\hat{H}_{w+} \ket{M(G_{w+})} = E_w \ket{M(G_{w+})} .$$

The ground states can be written as

$$\ket{M(G_{w+})} = \sum_j C_j \ket{\phi_j} = \sum_j C_j \ket{\psi_j} \otimes \ket{\phi_j} .$$

where $\ket{\psi_j}$ and $\ket{\phi_j}$ are the qubit and wire atom parts of the MIS solution $\ket{\phi_j}$ indexed with $j$. Note that the qubit state $\ket{\psi_j}$ (the combined state $\ket{\phi_j}$) is located in the Hilbert space whose size is $2^N$ ($2^{N-M}$), where $N$ and $M$ are the numbers of qubits of the target graph and wires, respectively. The MIS solutions of the wired graph are

$$M(G_{w+}) = \{ \ket{\psi_j} \otimes \ket{\phi_1}, \ket{\psi_j} \otimes \ket{\phi_2}, \ldots \} .$$

We introduce the projection operator, $P_H$, defined as

$$P_H \ket{\psi_j} = \ket{\psi_j} .$$

Mathematically, a Fock space with different qubit numbers is necessary, and yet it is safe to use the above notation for the MIS problems. The projection state is

$$P_H \ket{M(G_{w+})} = \sum_j C_j \ket{\psi_j} ,$$

and the corresponding solution set is

$$M(G_{w+}) = \{ \ket{\psi_1}, \ket{\psi_2}, \ldots \} .$$

where the bar notation is introduced to specify the projection. Some of the elements of $M(G_{w+})$ are not a solution of the MIS problem of $G_T$, being specified by the tilde notation. One can introduce the frustration function defined as $f(n_x, n_y) = n_x n_y$, where $n_x$ and $n_y$ are the number operator eigenvalues of the boundaries where a wire is connected. For an element of $M(G_{w+})$, the Rydberg blockade condition, $f(n_x, n_y) = 1$, can be tested, and a set with the condition is obtained, $\tilde{F}(G_{w+}) = \{ \ket{\psi_1}, \ket{\psi_2}, \ldots \}$. Then, one can introduce the second projection operator, $P_F = 1 - \sum_j \ket{\psi_j} \bra{\psi_j}$, and the final state is

$$\ket{M(G_T)} = P_F P_H \ket{M(G_{w+})} .$$

Then, the solution set can be written as

$$M(G_T) = M(G_{w+}) - \tilde{F}(G_{w+}) = \{ \ket{\psi_1}, \ket{\psi_2}, \ldots \} .$$

Note that our use of the frustration operator for post-selecting the solution set is closely related to the minor-embedding reduction in adiabatic quantum computing\(^3\), in which an Ising problem on a graph is dealt with using an embedded subgraph in a hardware-constraint graph along with an associated classical compilation.

**Data availability**

The data that support the findings of this study are available from Figshare, the public data repository at https://doi.org/10.6084/m9.figshare.19306640.v3. Source data are provided with this paper.

**Code availability**

The computer codes used to analyse the data of this study are available from Figshare, the public data repository at https://doi.org/10.6084/m9.figshare.19306640.v3.

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**Author contributions**

J.A. designed the project. M.K. and K.K. performed most of the experiments. M.K., K.K., J.H. and J.A. analysed and validated the data. E.-G.M. and J.A. wrote the manuscript. All authors have read, discussed and contributed to the manuscript.

**Competing interests**

The authors declare no competing interests.

**Additional information**

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