Quantum annealing of Cayley-tree Ising spins at small scales

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Significant efforts are being directed towards developing a quantum annealer capable of solving combinatorial optimization problems. The challenges are Hamiltonian programming and large-scale implementations. Here we report quantum annealing demonstration of Ising Hamiltonians programmed with up to \( N = 22 \) spins mapped on various Cayley tree graphs. Experiments are performed with a Rydberg-atom quantum simulator, in which rubidium single atoms are arranged in three dimensional space in such a way that their Rydberg atoms and blockaded strong couplings respectively represent the nodes and edges of each graph. Three different Cayley-tree graphs of \( Z = 3 \) neighbors and of up to \( S = 4 \) shells are constructed, and their ground-state phases and Néel’s order formations are probed. In good agreement with model calculations, the anti-ferromagnetic phase in regular Cayley trees and frustrated competing ground-states in a dual-center Cayley tree are directly observed. This demonstrates the possibilities of high-dimensional qubit connection programming in quantum simulators.

In recent years, quantum annealing has received significant attention because of their potentials in solving complex computational problems which are often intractable with current computational methods [1,2]. Quantum annealing is a procedure of making Hamiltonian \( H(t) \) of a quantum many-body system adiabatically evolve from \( \hat{H}_i \) to \( \hat{H}_f \),

\[
\hat{H}(t) = \hat{H}_i + \frac{t}{t_f} (\hat{H}_i - \hat{H}_f),
\]

so that the quantum state \( |\Psi(t)\rangle \) initially prepared in the ground state of the former reaches the ground state of the later. Quantum annealers are considered mostly with superconducting qubits [3–7] and trapped-ion qubits [8–11], aiming for various combinatorial optimization problems such as quantum simulations [12], classifications [13], planning [14], etc. While many efforts in quantum annealing are being focused on large-scale implementations [15,17] towards quantum speedup [18,21], here we explore the possibility of high-dimensional qubit connectivities. There are theoretical proposals emphasizing and thus utilizing qubit connectivities for NP-hard optimization problems: for example, the LHZ scheme [22, 23] proposed a quantum annealing architecture for all-to-all connectivities using local interactions; and quantum optimization protocols are considered, e.g., for maximum independent set problems utilizing the nature of long-range couplings especially in Rydberg-atom quantum simulators [24]. In the context relevant to the present work, Rydberg-atom quantum simulators [25, 26] draw attention, because of their high tunability in qubit connectivities [27,31] as well as many-body controllability in adiabatic processes [32,36].

In this work, we consider, as a prototypical fractal structures, Cayley tree graphs of neutral atom arrangements. Cayley trees are homogeneous and isotropic tree graphs of a fixed number of edges and no loop [37, 38]. Their infinite version is Bethe lattice widely used in various physics areas as a fundamental theoretical platform, often providing exactly solvable models in classical and quantum problems [39]. In experiments to be described below, we construct Cayley graphs of coordination number \( Z = 3 \) and shell number up to \( S = 4 \), as in Fig. 1, and use a Rydberg-atom quantum simulator to directly probe their Ising-Hamiltonian phases. In the following, we describe how these atomic Cayley trees are constructed and how their atom interactions are mapped to Cayley-tree graphs of Ising spins, before the result of quantum annealing of these Ising-graph Hamiltonians are analyzed.

Cayley trees of atoms in three-dimensional space. Neutral atoms (rubidium, \(^{87}\text{Rb}\)) are arranged in three-dimensional (3D) space with optical tweezers (far-off resonant dipole traps) [31]. As shown in Figs. 1(b–d), three different Cayley trees are constructed, which are \( G_{10} = (0s)(1s)^3(2s)^6 \), the three-shell \( (S = 3) \) Cayley tree having 10 atoms with one center atom, three second-shell atoms, and six third-shell atoms; \( G_{22} = (0s)(1s)^3(2s)^6(3s)^2 \), the four-shell \( (S = 4) \) Cayley tree having 22 atoms; and \( G_{14} = (0s)^2(1s)^4(2s)^8 \), the dual-center Cayley tree with two center atoms, four second-shell atoms, and eight third-shell atoms. In Cartesian coordinates, \( G_{10} \) can be two-dimensional, on the \( xy \) plane, as shown in Fig. 1(b), having the center atom at the origin and the second- and third-shell atoms respectively branched outward from previous-shell atoms. However, \( G_{22} \) and \( G_{14} \) require three-dimensional arrangements, because otherwise atoms on the outermost shells are too close. In that regards, we use three atom planes \((z = 0, \pm h)\) for \( G_{22} \) and \( G_{14} \), as shown in Figs. 1(c,d), so that all the last-shell atoms are well separated from each other. In \( G_{22} \), the last-shell branches are rotated by \( 2\pi/5 \) about the axes along previous branches and, in \( G_{14} \), some last-shell branches are rotated similarly. As-constructed atom arrangements are shown in Figs. 1(e–g) respectively for \( G_{10} \), \( G_{22} \), and \( G_{14} \).

When \( N \) atoms are coherently excited to a Rydberg
energy state, the Hamiltonian (in unit of $\hbar = 1$) is given in the van der Waals interaction regime \[34, 35\] by

$$
\hat{H}(t) = \frac{1}{2} \sum_{j=1}^{N} \left\{ \Omega(t) \hat{\sigma}_z^{(j)} - \Delta(t) \hat{\sigma}_x^{(j)} \right\} + \sum_{j<k} U_{jk} \hat{\sigma}_z^{(j)} \hat{\sigma}_z^{(k)}
$$

with $\Omega(t)$ the Rabi frequency, $\Delta(t)$ the detuning, and $U_{jk} = C_0 / |\vec{r}_{j} - \vec{r}_{k}|^6$ the inter-atom interaction, in which $\hat{\sigma}_{x,z}$ are Pauli operators defined for a pseudo spin 1/2 system composed of the ground state $|\downarrow\rangle$ and the Rydberg state $|\uparrow\rangle$ of each atom, and $\hat{n} = (1 + \hat{\sigma}_z)/2$. In one of the above atom arrangements of Cayley-tree graphs, non-connected couplings are between atoms separated more than the blockade radius ($r_b$), of at least 1/27 times smaller interactions than the connected couplings (of equal distance $d$), and thus ignorable. So, $U_{ij} = C_0 / d^6$ ($\equiv U$) for atom pairs $(i,j) \in E$, the edges (the nearest-neighbor pairs) of a graph $G$, and $U_{ij} = 0$ for others. The resulting $H$ is the Ising spin-glass Hamiltonian for $\Omega = 0$ and, as the ground-states of an Ising Hamiltonian depend on the specific atom arrangement $G$, finding such arrangement-specific ground-states for an arbitrary graph belongs to NP-hard problems \[40\].

**Quantum annealing of Cayley-tree Ising spins.** In our consideration, quantum annealing aims to find the antiferro-like ground states of Cayley-tree Ising spins, with time-varying laser parameters $\Omega(t)$ and $\Delta(t)$. Atoms are initially prepared in $|\downarrow\downarrow\cdots\downarrow\rangle$, the paramagnetic down-spin phase, which is the ground state of $H(0)$ under the conditions $\Omega(0) \ll U \ll -\Delta(0)$. The conditions for the final antiferro-like phase are given by $\Omega(t_f) \ll \Delta(t_f)$ and $\Omega(t_f) \ll U$. We choose $\Omega(t_f) = 0$ and $\Delta(t_f) \equiv \Delta \sim U$, so that more atoms favor up-spin states. Then, the target Hamiltonian $H_G$ for a graph $G \in \{G_{10}, G_{22}, G_{14}\}$ is given by

$$
\hat{H}_G = U \sum_{(j,k) \in E} \hat{n}_x^{(j)} \hat{n}_x^{(k)} - \frac{A}{2} \sum_{j=1}^{N} \hat{\sigma}_z^{(j)},
$$

which is in an Ising Hamiltonian form given by

$$
\hat{H}_G = J \sum_{(j,k) \in E} \hat{\sigma}_z^{(j)} \hat{\sigma}_z^{(k)} + h_{C}^{z} \sum_{j \in C} \hat{\sigma}_z^{(j)} + h_{V}^{x} \sum_{j \in V} \hat{\sigma}_z^{(j)},
$$

with $J = U/4$ the coupling, $h_{C}^{z} = 3U/4 - \Delta/2$ and $h_{V}^{x} = U/4 - \Delta/2$, the local fields, and $C$ and $V$ denoting the nodes in the core (inner shells) and valence (outermost) shell, respectively, of a Cayley-tree graph $G(E,C,V)$. Figure 2 shows the observed ground-states of the Cayley-tree Ising spins after quantum annealing. The quantum annealing is proceeded with three stages of time evolution. In the first stage ($0 < t < t_1$), the Rabi frequency is adiabatically turned on from $\Omega(0) = 0$ to $\Omega(t_1) = \Omega_0$ while the detuning $\Delta = -2\Omega_0$ is maintained for paramagnetic ordering ($|h_{C,V}^{z} \gg J|$). Then, in the second stage ($t_1 < t < t_2$), $\Omega = \Omega_0$ is maintained for state mixing and the detuning is swept from $\Delta(t_1) = -2\Omega_0$ to $\Delta(t_2) = 2\Omega_0$. In the final stage ($t_2 < t < t_f$), the detuning is maintained $\Delta = 2\Omega_0$ (for anti-ferromagnetic ordering, $0 < \Delta < 3U$) and the Rabi frequency is adiabatically turned off from $\Omega(t_2) = \Omega_0$ to $\Omega(t_f) = 0$.
The results are shown in Fig. 2, where the probabilities of spin configurations are plotted in a binary representation of the bare-atom basis, $|↓⟩=|0⟩$ and $|↑⟩=|1⟩$. The observed ground-state (the max-population state) of $H_{G_{10}}$ in Fig. 2(a) is $|↑↓↓↓↓⟩ = |2^9 + 2^6 + 2^4 + 2^3 + 2^2 + 2^1 + 2^0⟩ = |575⟩$. Likewise, the ground-state of $H_{G_{22}}$ is $|↓↑↑↑↑⟩ = |1839|103⟩$ in Figs. 2(b), and the ground-state of $H_{G_{14}}$ is doubly degenerate, $|↑↓↓↓⟩ = |4351⟩$ and $|↓↑↑↑⟩ = |8447⟩$ in Fig. 2(c). The corresponding ground-state atom images are shown in Figs. 2(d,e,f), respectively.

**Phase diagrams of Cayley-tree Ising Hamiltonians.** In order to understand the observed ground-state spin configurations, phase diagrams are obtained by comparing the energy values of Eq. (3) among all the possible spin configurations. The phase diagram for $G_{10}$ is shown in Fig. 3(a), which is the same as $G_{22}$. There are three ground-state configurations: the paramagnetic down and up phases (Phase I and II, respectively) and the anti-ferromagnetic phase (Phase III). In our consideration of positive coupling, $U > 0$, paramagnetic phases are expected at $\Delta \gg 0$ or $\Delta \ll 0$, and the anti-ferromagnetic phase in between. Note that in Cayley trees there are more spins on the valence shell than on the rest of the tree (the core shells). Therefore, the valence spins are all aligned either up or down depending upon $\Delta > 0$ or $\Delta < 0$, respectively, resulting in the $\Delta = 0$ phase boundary. For $\Delta < 0$, inner-shell spins also favor down, as their couplings, in terms of $U n(j)n(k)$ in Eq. (3), to outer-shell down spins are zero (so paramagnetic down spins, Phase I). For $\Delta > 3U$, the single-spin flipping energy ($\Delta$) is always higher than all adjacent anti-ferromagnetic couplings (of max $3U$), so all spins are up (paramagnetic up spins, Phase II). In between, $0 < \Delta < 3U$, the anti-ferromagnetic coupling is stronger, thus favoring the anti-ferromagnetic phase (Phase III) of shell-by-shell opposite spins. In short, the phase boundaries of Phase III, against Phases I and II, are determined by $E_{AFM} = E_{PM}$, respectively given by $\Delta = 3U$ and $\Delta = 0$, so the anti-ferromagnetic ordering occurs in the region $0 < \Delta < 3U$.

The phase diagram for $G_{14}$, the dual-center Cayley tree, is shown in Fig. 3(b). Phases I and II are paramagnetic phases, same as $G_{10}$ in Fig. 3(a), but Phase III is split to Phases IV and V, of respective center-spin configurations of $|↑↑⟩$ and $|↓↓⟩$. The phase boundary is given by $U = \Delta$, along which single-spin flipping cost equals the anti-ferromagnetic coupling energy. Experimental confirmation of the Phases IV and V is performed as in Fig. 3(c). Three different $G_{14}$ graphs, of respective edge lengths $d/r_b = 0.76, 0.86$, and $0.92$ (correspondingly $\Delta/U = 0.37, 0.74$, and $1.2$) are constructed and their probabilities of three low-energy states, $(|↑↑⟩ + |↓↓⟩)/\sqrt{2}$, $|↑↑⟩$, and $|↓↓⟩$, are respectively measured for the three $G_{14}$.
The IV-V phase boundary, $E(\uparrow\uparrow) = E(\downarrow\downarrow)$, is expected at $U(d_c = 0.89r_b) = \Delta$. The result in Fig. 3(c) shows that the max-populated state changes from $(\downarrow\downarrow) + (\uparrow\uparrow)/\sqrt{2}$ to $\uparrow\uparrow$, with $d$ across $d_c$ from the strong- to the weak-coupling regimes. Also, the first excited state also changes from $\downarrow\downarrow$ to $\uparrow\uparrow$ and then to $(\downarrow\downarrow) + (\uparrow\uparrow)/\sqrt{2}$, respectively at around $d/r_b = 0.79$ and 0.89. It is noted that the anti-symmetric state, $(\uparrow\downarrow) - (\downarrow\uparrow)/\sqrt{2}$, is forbidden by the Hamiltonian symmetry and that the higher-order long-range couplings ignored in Eq. $[2]$ play little role in the tested parameter region.

**Néel’s order formation dynamics.** The anti-ferromagnetic order formation is dynamically probed during the quantum annealing process. Figure 4 shows the time evolution of the Néel’s order defined by $O_N = -\sum_{i,j \in E}(\hat{\sigma}_i^{(i)}(t)\hat{\sigma}_j^{(j)}(t))/||E||$, along with the up-spin probabilities of each atom in $G_{10}$. The adiabatic order formation from the initial paramagnetic phase to the final anti-ferromagnetic phase is clearly observed with the snap-shot measurements. In comparison, a numerical calculation (solid lines) is performed with Lindblad master equations which take into account state-preparation-and-detection (SPAM) errors ($P(\downarrow \downarrow) = 0.18$, $P(\uparrow \downarrow) = 0.02$), individual dephasing ($\sim 36$ kHz) due to the spontaneous decay during Rydberg excitations, and collective dephasing ($\sim 3$ kHz) from laser phase noise $[41]$. The maximal Néel’s order of $O_N(t_f) = 0.48(2)$ is achieved for $G_{10}$, in accordance with the numerical calculation indicating that errors are largely due to the SPAM errors accumulated for $N = 10$ atoms. The calculation also suggests that the maximal Néel’s order before measurements was $O_N(t_f) = 0.82$ (with the ground-state probability of 61% through the quantum annealing).

**Experimental details.** The above experiments were performed with a Rydberg-atom quantum simulator previously reported elsewhere $[41]$. In the Rydberg quantum simulator, rubidium $^{87}{\text{Rb}}$ atoms are initially prepared in the hyperfine ground state, $|\downarrow\rangle = |5S_1/2, F = 2, m_F = 2\rangle$, and trapped with optical tweezers. A spatial light modulator (SLM, Meadowlark...
ODPDM512) is used to create the 3D array of optical tweezers and an electrically focus-tunable lens (EL-16-40-TC from Optotune) verifies the positions of captured atoms in each atom plane. The SLM is computer-programmed with weighted Gerchberg-Saxton (w-GS) algorithm so that the resulting electric field near each target site \((x, y, z)\) is created as \(E(x, y, z) = E_0 \sum_{X,Y} \exp(i(X,Y)) e^{-i\Omega t}\), where \(\Phi(X, Y)\) is the SLM phase pattern, \(T = 2\pi (xX + yY)/\lambda\), \(\pi \sigma(x^2 + y^2)/f^2\lambda\) is the transfer kernel, and \(X, Y\) are the SLM coordinates on the Fourier plane of the optical tweezers. The phase pattern \(\Phi\) is obtained with the w-GS condition, given by \(\Phi(X, Y) = \arg(\sum_{m} wE(x, y, z)e^{i\Omega t}/|E(x, y, z)|)\) with \(w\) the weighting factor optimized through adaptive iterations. The number of the w-GS iterations is about 5, taking about 20 ms time to generate an array of 50 tweezers. Deterministic rearrangement of atoms to target sites, about 20 \(\mu\)m apart from the initial atom reservoir, is performed with consecutive 45 frames of moving traps programmed with phase induction. Over 90% target-occupation probabilities are achieved in 900-ms reconfiguration time. Now with the atom array, the optical tweezers are temporarily turned off and the quantum annealing is proceeded. The atoms are excited to the Rydberg state, \(|\uparrow\rangle = |71S_{1/2}, m_J = 1/2\rangle\), via the off-resonant intermediate state, \(|i\rangle = |5P_{3/2}, F = 3, m_F = 3\rangle\). \(\Omega(t)\) and \(\Delta(t)\) in \(H(t)\) are programmed as \(\Omega(t)/\Omega_0 = 1 - (1 - t/t_1)\Theta(t_1 - t) - (t - t_2)/(t_2 - t)\) and \(\Delta(t)/2\Omega_0 = \Theta(t - t_2) - \Theta(t_1 - t) + (2t - t_1 - t_2)/(t_2 - t_1)\Theta(t - t_1)\Theta(t_2 - t)\) with a RF synthesizer (Moglabs XRF, 10 MHz) by frequency (780 nm) and amplitude (480 nm) modulations. Here, the times \(t_1 = 0.1t_f, t_2 = 0.9t_f,\) and \(t_f = (2\pi)3.2/\Omega_0\), are chosen for an adiabatic evolution optimized within coherence time. The modulation ranges are \(0 \leq \Omega(t) \leq \Omega_0\) and \(-2\Omega_0 \leq \Delta(t) \leq 2\Omega_0\), where the max Rabi frequency was \(\Omega_0 = \Omega_{780}/\Omega_{480}/(2\Delta') = 1.1 (2\pi)\) MHz given by \(\Omega_{780} = 75 (2\pi)\) MHz, \(\Omega_{480} = 19 (2\pi)\) MHz, and \(\Delta' = 600 (2\pi)\) MHz (the intermediate detuning). The van der Waals coefficient is \(C_6 = (2\pi)1004 \text{ GHz } \mu m^6\) for \(71S\) Rydberg-state atoms and the Rydberg blockade radius is \(r_b = (C_6/\Omega_0)^{1/6} = 9.8 \mu m\). In this case, the frequency error due to AC Stark shift is small, below 140 kHz, mainly caused by the 480-nm laser. After the quantum annealing, the optical tweezers are turned back on and the atom states are measured whether they survive \(|\downarrow\rangle\) or not \(|\uparrow\rangle\).

**Outlook.** While the possibilities of quantum annealing to quantum speedup are subjects of ongoing scientific controversies, there are many hopes to utilize the potentials of Rydberg-atom quantum simulators in large-scale implementations and high-dimensional configurability. With two-dimensional arrays, quantum annealing methods for NP-hard optimization problems on arbitrarily-connected graphs are proposed either with a typical Rydberg-atom quantum simulators or in an advanced setting utilizing dual atomic elements or multiple Rydberg levels. With three-dimensional arrays, atomic quantum wiring is proposed to directly implement programmable all-to-all connections of 1D Ising chains. It is hoped that 3D configurations of Rydberg atoms as shown in this paper shall be useful for efficient and programmable quantum annealing architectures for optimization problems.

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