Targeting Topological Optimization Problem: Sweeping Quantum Annealing

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Solving complex optimization problems by programmable quantum devices has attracted numerous efforts in recent years for seeking the potential advantages of the quantum computation. One practical route is to transfer the optimization problems to solving ground state of Ising models by quantum annealing. Due to the spin frustration that generically arises in this encoding, the algorithm design for the quantum annealing is crucial in order to fully exploit its computation power. Here we observe that topological defects decouple in the low-energy states of many frustrated (Ising) systems. The topological decoupling causes conventional quantum annealing (QA) algorithms failed thoroughly because the transition between topological sectors is difficult. The QA cannot lead the system to the topological sectors with lowest energy even through infinite time. We propose a sweeping quantum annealing (SQA) algorithm, and its substantial quantum speedup is demonstrated by comparing with other annealing methods. The SQA algorithm thus provides a generic recipe for resolving the topological decoupling in quantum optimization. This algorithm can be readily tested in experiments by superconducting qubits or Rydberg atomic systems.

Introduction.— Almost all quantum computing problems can be translated into computing the ground state of an encoded Ising type model [1–5]. Different from the thermal annealing (TA) making use of the thermal fluctuation, the QA utilizes the quantum fluctuation to approach the ground state [4, 6–9]. Following recent technological advancements in manufacturing coupled qubit systems, the QA algorithm can be embed into superconducting flux qubits [10–12]. Currently, QA computers, i.e., quantum annealer have also been commercialized, such as the D-wave machine, and it does show higher efficiency than classical computers in certain optimization problems [13–16].

On the other hand, the degree of quantum acceleration depends very much on the design of QA algorithm [17–19]. For example, confirmations of the superiority of QA have been obtained in systems such as the spin-1/2 disordered Ising ferromagnet, where the quantum annealing procedure, which attempts to follow the adiabatic quantum algorithm [19–21], works considerably better than classical TA in experiments [22, 23].

![Energy levels and configurations](image)

FIG. 1. Conventional optimization problems in glassy systems (a) and topological optimization problems in frustrated systems (b).

The realistic optimization problems can usually be classified into finding the ground states of Hamiltonian which is glassy, strongly frustrated or of both. In the past, much attention has been paid to the glassy case with the energy landscape shown in Fig. 1 (a), while the frustrated one in Fig. 1 (b) have been overlooked. As the complex topological defects which are robust to quantum fluctuations can emerge in low-energy states of many frustrated systems, it is realized that these emergent topological structures could deeply hinder the existing annealing algorithms, both TA and QA, inefficient. Therefore it is the time of finding generic annealing algorithms for such systems.

The difficult topological optimization problem has three characteristics as shown in Fig. 2 (a): 1) The minimum energies of many topological sectors are nearly equal. 2) The ground state is in the topological sector which occupies small Hilbert subspace. 3) There are some large topological sectors with nearly lowest energies, providing enough entropy to compete with the ground energy sector at finite temperatures. Then, the system under TA or QA prefer to stay in these large sectors.

In this manuscript, we consider a frustrated Ising model which can be easily implemented in the quantum annealer, such as D-Wave [24]. The model has fruitful topological features and it satisfies the above three characteristics. We focus on the comparison of the effectiveness of different annealing schemes to find the ground state among nearly degenerate topological sectors. While both QA and TA demonstrate their weakness on topological optimization problem as expected, we propose a generalized algorithm — sweeping quantum annealing (SQA) method — to solve the problem with better efficiency. Importantly, the SQA can be implemented easily in current quantum annealers and related experiments.

Microscopic spin Model.— To better understand the complex annealing process in a topological system, we study a sufficiently simple but not trivial system — the frustrated antiferromagnetic (AF) Ising model on a triangular lattice. The
emergent gauge fields and topological properties in this model have been well-studied [25–29]. Due to the antiferromagnetic interaction, in the low-energy Hilbert space, every triangle must be composed of two parallel and one antiparallel spins, such a local constraint is dubbed “triangle rule”. The “triangle rule” splits the low-energy Hilbert space into several topological sectors. The constraint-satisfying Hilbert space can be exactly mapped to a familiar dimer model [30–35] which is deeply related to programmable quantum simulator via Rydberg atoms [36, 37]. It is straightforward to see different topological sectors via $N_D = 0, 2$ and $4$ topological defects in Fig. 2 (b), (c) and (d). The defects number $N_D$ labels the related topological sectors. As well known, exactly at the classical Ising points of $h = T = 0$, the ground state has extensive degeneracy: any configuration that satisfies the triangle rule is a legitimate ground state, i.e., all the topological sectors are degenerate.

To clearly demonstrate the three characteristics of hard topology-optimization mentioned above, we introduce a small anisotropy for the nearest-neighbor (NN) AF Ising model to partially lift the degeneracy between different sectors,

$$H_A = J_x \sum_{\langle ij \rangle} \sigma_i^x \sigma_j^x + J_z \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z,$$

where $\sigma$ is the Pauli matrices, $\langle ij \rangle$ represent the nearest-neighbor sites on the horizontal bonds and the inter-chain bonds, respectively. With $J = 1$ and $J_x = 0.9$, the ground state of $H_A$ is a stripe-ordered phase [Fig. 2(b)] with the ground state energy exactly computable (for a $6 \times 6$ lattice, the energy for stripe state is $E_g = -39.6$). The model is simple enough with known ground state energy, yet it is non-trivial with the topological characteristics and very suitable to study the effectiveness of different annealing methods.

The ground state stripe phase in Fig. 2 (b) is composed of horizontal bonds connecting parallel spins and interchain bonds connecting antiparallel spins. Without breaking the local constraint of “triangle rule”, the number of horizontal antiparallel bonds is conserved in each row, and linking such antiparallel bonds on different chains will construct the one dimensional global (topological) defect [Fig. 2 (c) and (d)]. The topological sectors can be distinguished by the number of the topological defects, $N_D$, and changing it requires generating a pair of vortexes (constraint-breaking triangles) connected by defects [Fig. 2 (e)], letting them go around the connected boundary to meet and annihilate. Such process changes $N_D$ by two. However, exciting vortexes and pulling them apart is extremely hard at low temperatures, so that it is not easy to traverse topological sectors.

It is worth noting that spins on the corner of defects are flippable without energy cost, such as the red spin of Fig. 2 (c), after flipping the spin the corner on right side will be turned to left as shown by the dashed line. Therefore, the fluctuations introduced by both QA and TA can only deform the defects but cannot create/annihilate them. In essence, the optimization problem is an annealing problem to find the optimal topological sectors in Fig. 2 (a). In this case, the number of states in a topological sector increases with the increase of $N_D$, so the stripe configuration of the ground state is hard to be reached in Hilbert space as one needs an annealing algorithm that can both tunnel through different topological sectors and reduce the energy.

**Traditional thermal annealing and quantum annealing.—**

The thermal annealing (TA) scheme is to slowly reduce the temperature of $H_A$ from a region where local minima can be easily escaped and the system can gradually evolve to ground state. We simulate the thermal annealing process by using the Metropolis Monte Carlo [1, 39] with local spin flips. The Boltzmann constant is set to $k_B = 1$ for convenience, and we perform thermal annealing through linearly decreasing temperature from $T = 5.00$ to $T = 0.05$ with cooling interval $\Delta T = 0.05$. In contrast, quantum annealing (QA) requires the introduction of the quantum fluctuation, turning the Hamiltonian into $H_QA = H_A + h(t) \sum_i \sigma_i^z$ with the transverse field $h(t)$ slowly reduced to zero so that the original Ising Hamiltonian $H_A$ is recovered at the end of the process. The quantum annealing is implemented by utilizing the quantum Monte Carlo (QMC) simulation [39–43], and we adopt the stochastic series expansion (SSE) method [2–4, 47, 48] to avoid the Trotter discretization error [8, 40]. The QMC schemes have been successfully employed in many previous works on quantum Ising models [27, 28, 49]. Similar to thermal annealing, we carry out quantum annealing with linearly decreasing transverse field from $h = 5.00$ to $0.00$ with annealing interval $\Delta h = 0.05$, and the temperature $T = 0.05$ is low enough to ignore the thermal effect. In order to compare thermal and quantum annealing, we study how the energy $E$ evolves under the same annealing time, in the unit of Monte Carlo step (MCS).
We have simulated the system with sizes $6 \times 6$ with periodic boundary conditions and parallelized the simulations on 64 independent Markov chains to achieve better statistics.

As shown in Fig. 3 (a), the QA turns out to have poor performance with energy difference $\Delta E = E - E_g \approx 5$. This can be qualitatively understood from the phase diagram of original AF transverse field Ising model on triangular lattice [25–28]. The annealing path of TA is mostly inside the disordered phase whereas the path of QA experiences an extra clock-ordered phases. The clock phase is actually the largest topological sector with most degrees of freedom as the blue sector shown in Fig.2 (a). In fact, the clock phase can be seen as the configuration with most topological defects and corners, and all the corners are resonant. It makes the quantum fluctuations (kinetic terms) optimal within this sector and the system will not be able to reach the lowest energy topological sector, that is the difficulty for the topological optimization. Moreover, the transition between different topological sectors is a difficult first order phase transition in fact [29], the different minimum states with different good quantum number (defect number) cross at certain parameter points.

To overcome such difficulty in QA, we have also tried the quantum annealing with inhomogeneous field $H_{QA-h} = H_A + h_i(t) \sum_i \sigma_i^y$ with site-dependent $h_i(t)$. The disordered magnetic field is suggested to weaken the effect of phase transition and improve the efficiency of quantum annealing [53–57]. At initial time $t=0$, we randomly generate values from 0 to 10 to for each $h_i$. Then all $h_i$ are linearly reduced to 0 in the QA process. We denote such annealing as “QA-h” in Fig. 3 (a). However, it turns out that our constrained optimization problem exceeds the capability of random quantum fields [53–57], the result of QA-h looks similar to QA without obvious improvement. It is more intuitive to understand that the external quantum tunneling term prefers the sector with more states, so the quantum term is more willing to stay in the clock phase, in which there are a lot of flippable spins in low-energy configurations.

**Sweeping quantum annealing algorithm.** As discussed above, the topological optimization problems usually involve non-local excitations and require global operations. Since the system can easily reach the global minimum intuitively if we can change the boundary condition. It inspires us to invent the sweeping quantum annealing algorithm (SQA).

A feasible algorithmic scheme on a quantum annealing platform is to do additional annealing with a large transverse field on edge. Intuitively, a large transverse field can polarize the spin to the x-axis, acting as if shearing the coupling bond apart. A great advantage is that the strength of the transverse field can be easily and continuously adjusted by laser frequency in experiment. We scan all the “edges” along a certain direction with strongly annealing transverse field [Fig. 3 (b)], which is expected to achieve the effect across topological sectors. The specific plan is as follows: 1) Keep the traditional quantum annealing process as mentioned above, that is, decreasing the $h$ slowly down till zero. 2) Divide the whole process into $L$ (system length) parts. In every part, add a extra strong transverse field on “edges” in order and reduce the field strength slowly to $h(t)$. $h(t)$ is the strength of the traditional QA at the end of this part. From Fig. 3 (a), we can see an obvious advantage of SQA to arrive at ground state quickly. The detailed pseudo-code protocol of SQA is shown in the Supplemental Materials (SM) [39].

In order to better understand the working mechanism of SQA, we give a physical explanation via a picture of flippable topological defects. Let’s decompose the SQA into a sequence of cut-and-glue steps. In principle, we can cut the system to artificially create an open boundary [Fig. 3 (c)]. In order to allow the topological defect [58–60] to pass through the boundary and disappear to change the topology, we need to make the spins at the open boundary flippable with nearly 0 energy cost. We change the coupling strengths of the bonds at the boundary to a different value $J_e$. The corresponding energy shift of one edge spin flipping process, e.g., the collapsed spin-up and spin-down of blue spin on edge in Fig. 3 (c) is $2(J_e - J_s)$. In order to soften the boundary, we set $J_e = J_s/2$ to make spin more flippable. After equilibrating the system with open boundary conditions for some time, the edges need to be glued to restore the original boundary conditions when...
utilizing the quantum annealing.

After one cut-and-glue step, we move to another position and repeat until all edges have been swept. We call this scheme as open boundary quantum annealing (OQA), more details of OQA can be seen in SM [39] The efficiency of OQA should be very close to SQA and this is indeed shown in Fig. 3 (a), that their effects are really the best of all. SQA is better than OQA perhaps because the $J_\perp$ we set in OQA can not let the spin to be flipped with exact 0 energy cost, but SQA can achieve such zero energy cost. Moreover, SQA can be realized in experiment easily via tunable laser or arbitrary waveform generator [61–63].

FIG. 4. (a) The proportion of ground state sector as a function of the annealing time with different methods. (b) The proportion of all topological sectors as a function of the annealing time with different methods.

The physical reason of the superior behavior of SQA in the topological frustrated optimization problem is that it effectively removes topological defects in the systematic sweeping. As demonstrated in Fig. 4 (a), the proportion of $N_D = 0$ sector (stripe phase) are increasing with annealing time except for QA and QA-h. After $t$/MCS $\approx 10^7$, the increasing rate of SQA surpasses the TA, and SQA exhibits the best optimization results. Furthermore, the proportion of different topological sectors are shown in Fig. 4 (b). The conventional QA and QA-h are stuck in $N_D = 4$ sectors, which reveals the reason for their inefficiency. Although the TA can also change the topological sectors due to the creation of pairs of vortex excitations in Fig. 2 (b), clearly the best of all annealing schemes is the SQA (OQA is very close to SQA, but quite artificial) which can straightforwardly change the topology of the system at any position.

In order to strengthen the evidences of effectiveness and universality of SQA, we simulate another difficult topological optimization problem of a fully frustrated Ising system on square lattice in SM [39]. In addition, the algorithm effect of different size systems is also present in SM [39].

Discussions.—In realistic optimization problems, emergent topology exist ubiquitously. For such topological optimization problems, there is still a lack of systematic quantum computing research. In this work, we find that the emergent topological properties in frustrated Ising systems greatly reduce the efficiency of both conventional thermal and quantum annealing. Borrowing the idea of changing topology by cutting and gluing the system, we invent a generalized algorithm — the sweeping quantum annealing method to solve these problems with huge quantum speedup. Moreover, the SQA can be easily implemented in realistic quantum simulation experimental platforms because the global transverse field term can be controlled finely by tunable laser or arbitrary waveform generators [24, 50–52, 61–65]. After comparing with conventional quantum and thermal annealing algorithm, we find that this algorithm presents high efficiency and validity while other annealing schemes fail. The sweeping quantum annealing algorithm therefore opens up an effective and innovative way for the application of quantum computing on realistic topological optimization problems. It will be of interests to study the effectiveness of SQA under noises and dissipations [66, 67] which commonly exist in the quantum annealer.

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SUPPLEMENTAL MATERIALS

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Pseudo-code of SQA

The details of sweeping quantum annealing (SQA) algorithm can be written via a pseudo code as Table I.

| TABLE I. The pseudo-code demonstrating the sweeping annealing procedure. |
|---|
| 1. **Define** steps ! annealing steps in each \( \Delta h \) window. |
| 2. **Define** \( n = L \) ! # of cutting position. |
| 3. **Set** \( n_s = \text{steps}/n \) ! # of annealing steps for gluing. |
| 4. **For** \( h = h_{\text{max}} : = \Delta h : 0 \) ! annealing loops |
| 5. **For** \( i_e = 1 : n \) ! sweeping loops |
| ! ———-Cutting Process———- |
| 6. **Set** \( h_e = h_{\text{max}} \) ! \( h_e \) denote h acts on the edge. |
| ! ———-Gluing Process———- |
| 7. **Set** \( \Delta h_e = (h_{\text{max}} - h)/n_s \) ! the increment of gluing. |
| 8. **For** \( i_g = 1 : n_s \) ! gluing loops |
| 9. **One** annealing step with QMC |
| 10. **Set** \( h_e = h_e - \Delta h_e \) ! smoothly restoring the boundary condition |
| 11. **End** |
| 12. **Move to next cutting position** |
| 13. **End** |
| 14. **End** |

Pseudo-code of OQA

The details of open boundary quantum annealing with sweeping \( L \) open boundaries (OQA) can be written via a pseudo code as Table II.
### TABLE II. The pseudo-code demonstrating the sweeping annealing procedure.

| Step | Description |
|------|-------------|
| 1.   | Define steps \( \text{! annealing steps in each } \Delta h \text{ window.} \) |
| 2.   | Define \( n = L \) \( \text{! # of cutting position.} \) |
| 3.   | Set \( n_s = \text{steps}/n \) \( \text{! # of annealing steps for gluing.} \) |
| 4.   | For \( h = h_{\text{max}}, -\Delta h : 0 \) \( \text{! annealing loops} \) |
| 5.   | For \( i_s = 1 : n \) \( \text{! sweeping loops} \) |
| 6.   | Set \( J_x = 0, J_e = J_x/2 \) \( \text{! x- denote the bonds disjointed.} \) |
| 7.   | Set \( \Delta J_x = J_x/n_s, \Delta J_e = (J - J_x/2)/n_s \) \( \text{! the increment of gluing.} \) |
| 8.   | For \( i_g = 1 : n_s \) \( \text{! gluing loops} \) |
| 9.   | One annealing step with QMC |
| 10.  | Set \( J_x = J_x + \Delta J_x; J_e = J_e + \Delta J_e \) \( \text{! smoothly restoring the boundary condition} \) |
| 11.  | End |
| 12.  | Move to next cutting position |
| 13.  | End |
| 14.  | End |

#### Classical Monte Carlo for thermal annealing

We use Metropolis Monte Carlo [1] which flip single spin to simulate Eq. (S3) thermal annealing. Its general process is as follows: assume we have reached configuration \( C_1 \) with energy \( E_1 \). Firstly we choose a spin randomly and flip it to get a new configuration \( C_2 \) with energy \( E_2 \). We use the acceptance probability \( P = \min(e^{-\beta(E_2 - E_1)}, 1) \) to determine whether to update the system to configuration \( C_2 \), otherwise we keep configuration \( C_1 \). For the thermal annealing process, we do the Monte Carlo simulation from \( T = 5 \) to \( T = 0.05 \), the decreasing interval is \( \Delta T = 0.05 \), and MCS of every interval is fixed.

#### Quantum Monte Carlo for quantum annealing

For the quantum annealing in this paper, we use a quantum Monte Carlo (QMC) method with stochastic series expansion (SSE) algorithm[2–4]. In this method, the evaluation of partition function \( Z \) is done by a Taylor expansion, and the trace is taken by summing over a complete set of suitably chosen basis.

\[
Z = \sum_{\alpha} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} (\alpha|(-H)^n|\alpha) \quad (S1)
\]

By writing the Hamiltonian as the sum of a set of operators whose matrix elements are easy to calculate \( H = -\sum_i H_i \) and truncating the Taylor expansion at a sufficiently large cutoff \( M \), we can further obtain

\[
Z = \sum_{\alpha} \sum_{\{i_p\}} \frac{\beta^n (M - n)!}{M!} \langle \alpha | \prod_{p=1}^{n} H_{i_p} | \alpha \rangle \quad (S2)
\]

To carry out the summation, a Markov chain Monte Carlo procedure can be used to sample the operator sequence \( \{i_p\} \) and the trial state \( \alpha \). One step of the update process contains diagonal update and off-diagonal update. In the diagonal update, the diagonal operators are inserted into and removed from the operator sequence. Meanwhile, in the off-diagonal update, the diagonal and off-diagonal operators can be converted into each other. In the quantum annealing process, we decrease the transverse field from \( h = 5.00 \) to \( h = 0.00 \), with a decreasing interval \( \Delta h = 0.05 \). A tiny residual field is kept to facilitate the update process.
Annealing results of different sizes

We also simulate TA, QA and SQA on $4 \times 4$ and $8 \times 8$ triangular lattice to see the corresponding annealing effects. As can be seen from the Fig.S1[(a) for 4x4, (b) for 8x8], the leadership of SQA does not change because of the lattice size. Besides, we can also intuitively feel that larger size needs longer annealing time. Moreover, the superiority of SQA becomes more obvious in larger size.

Fully frustrated Ising model on square lattice

Similar to the frustrated Ising model on triangular lattice in main text, we give a fully frustrated Ising model on square lattice. The Hamiltonian to be annealed is as following:

$$H_A = \sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z$$

$i,j$ here mean the positions of spins of nearest neighbors. As in Fig.S2 (a), the thick gray bonds are antiferromagnetic (AFM) (set $J_{ij} = 1$), and the thin black bonds are ferromagnetic (FM)(set $J_{ij} = -1$). What’s more, we set the links crossed by dimers a little weaker ($J_{ij} = 0.9$ for AFM and -0.9 for FM) to let dimers condensed on the corresponding positions. The low energy fully frustrated rule is equal to the condition that there must be and only be one dimer on every site of dual lattice, which contains an emergent gauge field constraint. The anisotropy make the staggered sector become the lowest energy one. Therefore, the model has similar topology annealing problem as in Fig.1 of main text.

We compare TA, QA and SQA similarly as in main text. The SQA is also the best scheme as Fig.S2 (b) shown.

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FIG. S2. (a) A fully frustrated Ising model on square lattice. The thick gray bonds are antiferromagnetic, and the thin black bonds are ferromagnetic. The spins of one bond is not low energy that creates a dimer on its dual bond. The low energy fully frustrated rule is equal to the condition that there must be and only be one dimer on every site of dual lattice. We set the links crossed by dimers a little weaker to let dimers condensed on the corresponding positions. Therefore the staggered sector becomes the lowest energy one. (b) The energy is computed for 6 × 6 system and the true ground state energy is denoted by the grey dashed line.