Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary material: Vacancies in graphene: an application of adiabatic quantum optimization

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1 DW_2000Q_6 hardware

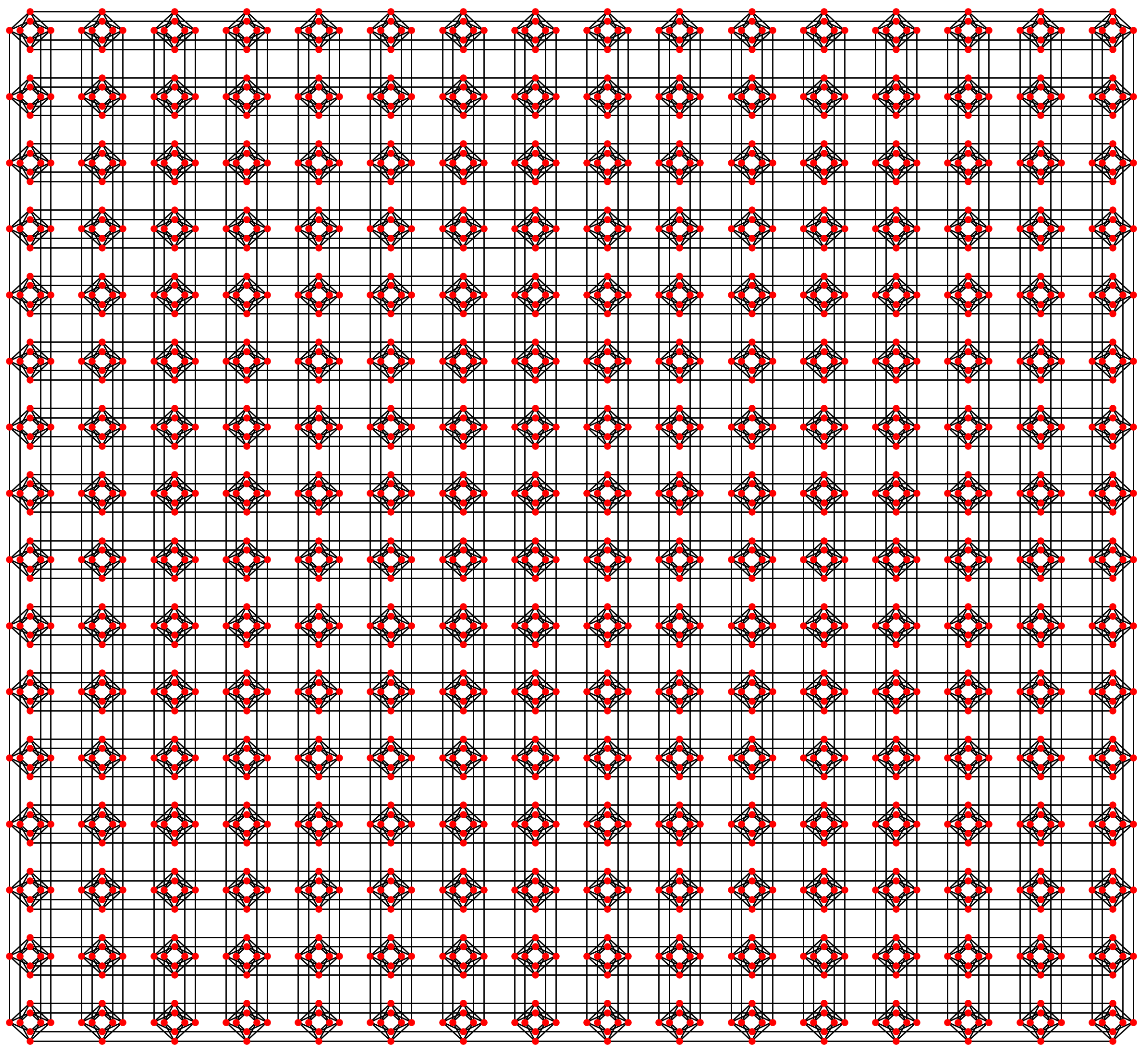

Fig. 1 Schematic representation of the fully Chimera graph of DW_2000Q_6 (DW2Q6) developed by D-Wave System Inc. and used in this work. Red circles represent qubits while lines represent couplings between qubits. Each qubit can be coupled to a maximum of six other qubits.

In D-Wave quantum annealers, physical qubits are arranged in a Chimera graph $C(\mathscr{V},\mathscr{E})$ topology; the one for DW_2000Q_6 (DW2Q6) has N=2041 qubits, and each qubit can coupled with maximum other six qubits (Fig. 1). Usu-

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ally, a problem represented by a QUBO is mapped into a graph $G(\mathscr{V},\mathscr{E})$ that has higher connectivity with respect to the $C(\mathscr{V},\mathscr{E})$. This is also the case of our work. The point, then, is mapping (through the so-called minor embedding process) the “logical problem" on the physical DW2Q6 hardware[1,2]. This introduce the concepts of “physical qubits", meaning a set of linked (logical) qubits acting as a single (physical) qubit. D-Wave’s API provides a tool called `minorminer` which heuristically searches for the optimal (minor)embedding[3]. `minorminer` searches for the minimum length of each embedding chain, as shorter chains are less prone to breaking into domains of physical qubits with opposite spin orientations. Physical qubits belonging to the same logical qubit are strongly coupled by an intra-chain bias (J_F). The J_F is important as it affects the time-dependent energy spectrum in the adiabatic evolution and determines the ability of the chain to act as a single variable; the J_F bias should be strong enough to avoid chain-breaking without dominating the dynamics. Ideally, once the J_F is set correctly, all solutions returned by DW2Q6 would correspond to valid logical solutions, where all the physical qubits within a logical qubit would have the same spin. Because of the probabilistic nature of quantum annealing, as well as noise from different sources, often some percentage of solutions have broken chains. Three approaches are possible to deal with broken chain solutions. The first method is simply discarding these solutions; the second one, so-called “majority voting", assigns to the logical qubit the spin with the major vote within the physical qubits of the chain; the last one is to go through the broken chains one by one and select the setting that minimizes the energy of the QUBO. The approach used in this work is the first one.

2 Time To Solution: quantum annealing vs simulated annealing

The time performance of DW2Q6 is assessed by computing the time to get the solution with probability 99%:

$$\mathrm{T}_{99} = \frac{ln(1-0.99)}{ln(1-\mathrm{P}_{gs})}T$$

where T is the annealing time and P_{gs} is the probability of finding the correct ground state at annealing time T. Because the best T is different from one embedding to another, it is not possible to select a T that allows top performance for all the embeddings. According to this, we have evaluated T_{99} using the default T=$20\mu s$. The performance of DW2Q6 has been compared also with simulated annealing as implemented in D-Wave Ocean SDK[4]. Following the literature[5,6], the time to solution for SA reads as:

$$\mathrm{TTS} = N^2\frac{ln(1-0.99)}{ln(1-\mathrm{P}_{gs})}\tau_s n_s$$

where N is the number of logical variables of the problem, n_s is the number of sweeps, and $\tau_s = 1/f_{SA}$ the time required to perform a single sweep (f_{SA} is the number of spin updates per unit time). Because the SA algorithm performs one spin flip per time step and the clock rate of our cpu is 2.4 GHz, $f_{SA} = 2\,\mathrm{ns}^{-1}$. The chosen SA annealing schedule β is comparable to the one of DW2Q6.

3 Results by Quantum Annealing: penalty constant and intra-chain coupling

In this section, we report a comparison in the performance of DW2Q6, measured as probability of finding the correct ground state (P_{gs}) as a function of the intra-chain coupling J_F. The P_{gs} has been computed for different values of the penalty cosntant p (see Eq. 1, main text). The coefficients in front of the penalty functions have a main role in tuning the gap between the ground state and the first excited state of the QUBO[7,8]. Indeed, we notice that the P_{gs} for quantum annealing decreases with the increasing of p (Fig. 2), while the trend and the best choice for the J_F do not change with p.

Notes and references

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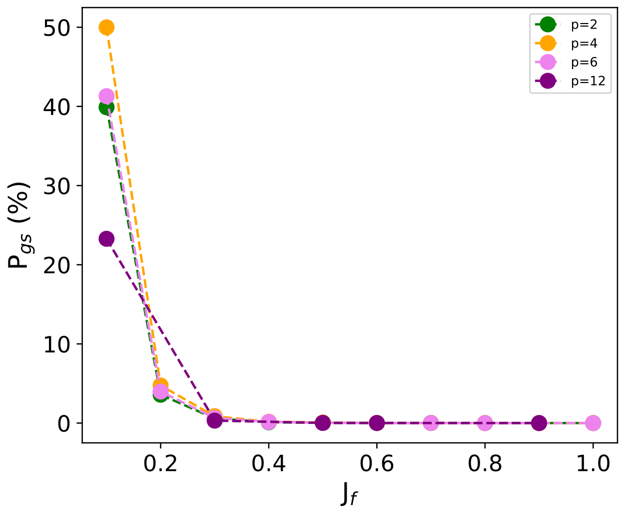

Fig. 2 Probability of finding the correct ground state (P_{gs}) as a function of the intra-chain coupling (J_F) for different penalty constant p (see Eq.1, main text). Only solutions with unbroken chains are counted. Runs are performed using 100 spin reversal operations. For each run on DW2Q6 the embedding was chosen randomly.

8 V. Choi, *Quantum Information Processing*, 2020, **19**, year.