From Quantum Technologies to hardcore Graph Theory

Robert Kooij
15 June 2023

Lecture for QCE Department

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Introduction

- Progress in quantum technologies
  - Hardware
  - Software
- When do we have quantum advantage?
- Accelerate computation of a hard, real-world problem
  - Diversity of quantum HW and SW
- Need for application level quantum benchmark

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Introduction

- Component-level benchmarks
  - Fidelity of quantum gates
  - Number of qubits
- (Sub)system-level benchmarks
  - Quantum Volume
  - Circuit Layer Operations Per Seconds (CLOPS)
- Application-oriented benchmarks
  - QED-C (Quantum Economic Development Consortium) Benchmark
  - Q-Pack TU Delft

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Introduction

- Q-Score: metric proposed by Atos
  - Application-centric
  - Hardware-agnostic
  - Scalable
- Largest problem size N for which a quantum device significantly outperforms a random algorithm at solving an NP-hard problem: **Max Cut problem**

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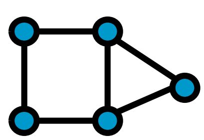
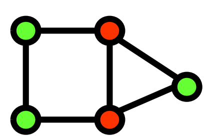
Overview

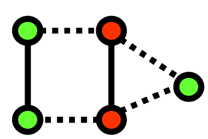
- Max Cut problem
- Q-Score
- Quantum Annealing
- Q-Score for a Quantum Annealer
- Gaussian Boson Sampling
- Max Clique problem
- Other NP-hard problems
- Other connections with Graph Theory
- Wrap-up

Max Cut problem



Partition nodes into two sets

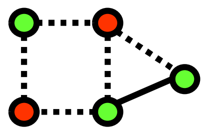




- Cut: number of links between the two sets

Max Cut problem

- Max Cut: partition with maximum number of links



- Max Cut problem is NP-hard

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Q-Score

- Largest problem size N for which a quantum device significantly outperforms a random algorithm at solving the **Max Cut problem**

- Needed: a class of graphs for which we have:
  - An (asymptotic) expression for C_{max}
  - A fast random algorithm to determine C_{rand}

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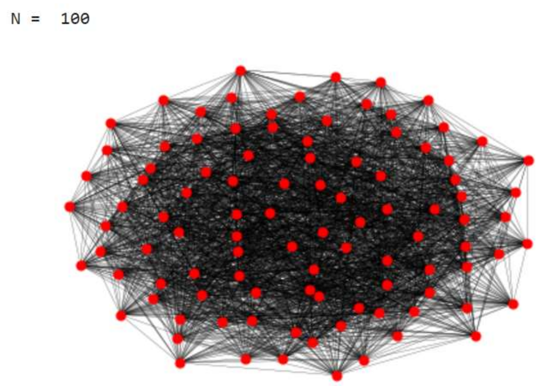
Q-Score

- Erdős–Rényi graph ER(N, 1/2)
  - Random graph on N nodes
  - Link probability p = 1/2



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Q-Score

- ER(N, 1/2)   An (asymptotic) expression for C_{max}

The Annals of Probability
2017, Vol. 45, No. 2, 1190–1217
DOI: 10.1214/15-AOP1084

EXTREMAL CUTS OF SPARSE RANDOM GRAPHS

BY AMIR DEMBO[1], ANDREA MONTANARI[2] AND SUBHABRATA SEN[3]

$$C_{max} \approx \frac{N^2}{8} + 0.178N\sqrt{N}$$

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Q-Score

- ER(N, 1/2)   A fast random algorithm to determine C_{rand}

Random partition: two random sets of N/2 nodes

$$C_{rand} \approx \frac{N^2}{8}$$

Q-Score

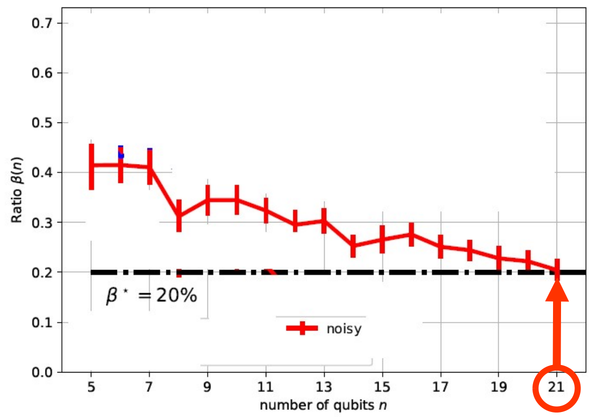
- Algorithm: for increasing N do:
  - Make M realisations of G(*N,1/2*)
  - Run Max Cut algorithm for every graph
  - Determine average Max Cut C(N)
- Check whether this average has "sufficiently" high score

$$\beta(N) = \frac{C(N) - C_{rand}}{C_{max} - C_{rand}} > \beta^* = 0.2$$

- Q-score: highest N for which $\beta(N) > \beta^*$

Q-Score

- ATOS: Quantum Approximate Optimization Algorithm (QAOA)
- Simulation of their own quantum device (gate based)



Q-score = 21

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Quantum Annealing

- Quantum version of Simulated Annealing
  - Find global minimum of a given objective function
  - Minimize a Ising spin Hamiltonian

$$\mathcal{H}(\mathbf{h}, \mathbf{J}, \boldsymbol{\sigma}) = \sum_i h_i \sigma_i + \sum_{i<j} J_{ij} \sigma_i \sigma_j$$

- **h**: external field
- **J**: spin coupling interactions
- σ_i: spin values $\in$ {-1,1}

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Quantum Annealing

- 5000+ qubits
- Cloud interface (1 minute free QPU time)

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Quantum Annealing

- Ising Hamiltonion <-> QUBO
- Quadratic Unconstrained Binary Optimization

Minimize $y = \mathbf{x}^T Q \mathbf{x}$

$\mathbf{x}$ = N-dimensional binary decision vector
Q = NxN symmetric constant matrix

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Quantum Annealing

- Many Combinatorial Optimization problems can be formulated as a QUBO

frontiers in PHYSICS
REVIEW ARTICLE
published: 12 February 2014
doi: 10.3389/fphy.2014.00005

Ising formulations of many NP problems

*Andrew Lucas**

Lyman Laboratory of Physics, Department of Physics, Harvard University, Cambridge, MA, USA

- These problems can be programmed on D-Wave!

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Q-Score for a Quantum Annealer

TNO

- Q-Score for D-Wave

2022 IEEE International Conference on Quantum Software (QSW)

Evaluating the Q-score of Quantum Annealers

Ward van der Schoot, Daan Leermakers, Robert Wezeman, Niels Neumann, Frank Phillipson

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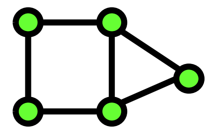
Q-Score for a Quantum Annealer

- QUBO for Max Cut

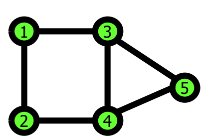


- Binary variables x_i
  - $x_i = 1$: node i belongs to set 1
  - $x_i = 0$: node i belongs to set 2

- $x_i + x_j - 2x_ix_j = 1 \Leftrightarrow$ link (i,j) is in the cut
- $x_i + x_j - 2x_ix_j = 0 \Leftrightarrow$ link (i,j) is not in the cut

Q-Score for a Quantum Annealer

- Maximize $y = \sum_{(i,j)\in E} (x_i + x_j - 2x_ix_j)$



$$y = x_1+x_2\text{-}2x_1x_2 + x_1+x_3-2x_1x_3$$
$$x_2+x_4\text{-}2x_2x_4+ x_3+x_4\text{-}2x_3x_4$$
$$x_3+x_5\text{-}2x_3x_5 + x_4+x_5\text{-}2x_4x_5 =$$

$$2x_1+2x_2 + 3x_3 + 3x_4 +2x_5 \text{-}2x_1x_2\text{-}2x_1x_3\text{-}2x_2x_4\text{-}2x_3x_4\text{-}2x_3x_5\text{-}2x_4x_5 =$$

$$2x_1^2 + 2x_2^2 + 3x_3^2 + 3x_4^2 + 2x_5^2\text{-}2x_1x_2\text{-}2x_1x_3\text{-}2x_2x_4\text{-}2x_3x_4\text{-}2x_3x_5\text{-}2x_4x_5=$$

Q-Score for a Quantum Annealer

$$(x_1\, x_2\, x_3\, x_4\, x_5)\begin{pmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 2 & 0 & -1 & 0 \\ -1 & 0 & 3 & -1 & -1 \\ 0 & -1 & -1 & 3 & -1 \\ 0 & 0 & -1 & -1 & 2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{pmatrix}$$

$$\mathbf{x} = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad \Rightarrow \quad y = \mathbf{x}^T Q \mathbf{x} = 5$$

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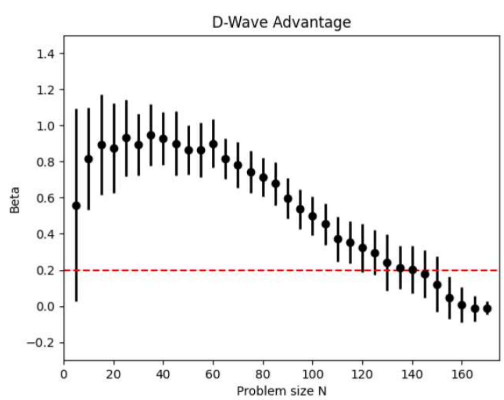
Q-Score for a Quantum Annealer

- Results TNO paper

Approach	Q-score
Tabu search	2,300
Simulated annealing	5,800
D-Wave Advantage	140
D-Wave 2000Q	70
Hybrid solver	12,500

D-WAVE QUBO solvers
(60 seconds time limit)



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Q-Score for a Quantum Annealer

- Q-Score determined for
  - Gate based device (ATOS)
  - Quantum Annealer (D-Wave)
- Other physical quantum devices exist

Gaussian Boson Sampling

- Available quantum computers
  - Diversity of physical platforms
    - Superconducting qubits
    - Trapped ions
    - Photonics
    - Quantum annealers
    - Rydberg atoms
    - …

Gaussian Boson Sampling

- Special-purpose photonic platform
  - Gaussian Boson Sampling
  - Sampling tasks intractable to classical computers

XANADU
Photonic Quantum Computing

QuiX QUANTUM

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Gaussian Boson Sampling

- Symmetric square matrix A (representing graph G)
  → can be encoded into GBS device

- State of GBS correlates with Hafnian of A

- Hafnian of A: = # perfect matchings of G

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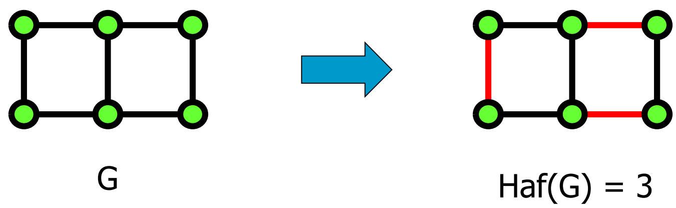
Gaussian Boson Sampling

- Perfect matching: set of links such that each node is adjacent to exactly one link



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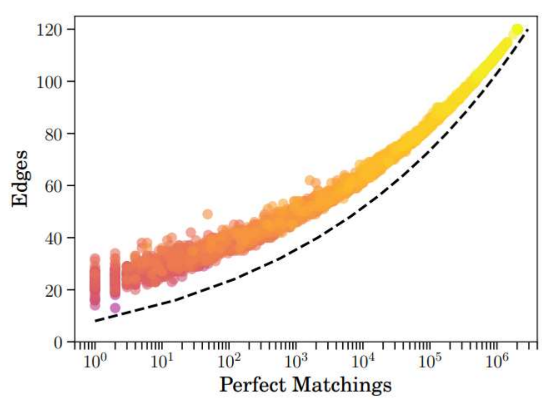
Gaussian Boson Sampling

- # perfect matchings correlates with link density



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Gaussian Boson Sampling

- Subgraph sampling → high probability to sample a dense subgraph
- Can be explored for efficient algorithms for
  - Max Clique
  - K-densest subgraph identification
  - Graph similarity algorithms

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Gaussian Boson Sampling

Applications of near-term photonic quantum computers: software and algorithms

Thomas R Bromley[1], Juan Miguel Arrazola[1], Soran Jahangiri[1], Josh Izaac[1], Nicolás Quesada[1], Alain Delgado Gran[1], Maria Schuld[1], Jeremy Swinarton[1], Zeid Zabaneh[1] and Nathan Killoran[1]

Published 12 May 2020 • © 2020 IOP Publishing Ltd

Quantum Science and Technology, Volume 5, Number 3

Citation Thomas R Bromley *et al* 2020 *Quantum Sci. Technol.* **5** 034010

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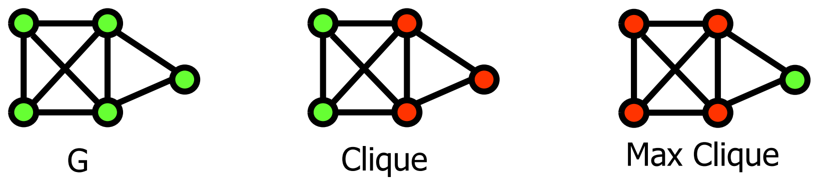
Max Clique problem

- Clique = complete subgraph in G
- Max Clique = largest clique in G



- Max Clique problem is NP-hard

Max Clique problem

TNO
- proposed Q-Score+

- Largest problem size N for which a quantum device significantly outperforms a random algorithm at solving the **Max Clique problem**
- Implementable on
  - Gate based devices
  - Quantum annealer
  - Gaussian Boson Sampling device

Max Clique problem

- Algorithm: for increasing N do:
  - Make M realisations of G(N,1/2)
  - Run Max Clique algorithm for every graph
  - Determine average Max Clique M(N)
- Check whether this average has "sufficiently" high score

$$\gamma(N) = \frac{M(N) - M_{rand}}{M_{max} - M_{rand}} > \gamma^* = 0.2$$

- Q-score+: highest N for which $\gamma(N) > \gamma^*$

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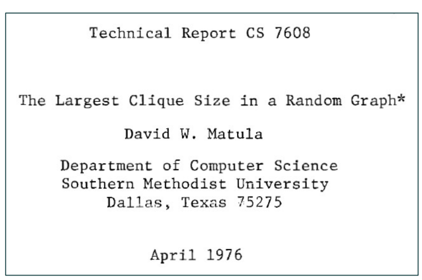
Max Clique problem

- For ER(N,1/2) we need:
  - An (asymptotic) expression for M_{max}
  - A fast random algorithm to determine M_{rand}

M_{max} →


Technical Report CS 7608

The Largest Clique Size in a Random Graph*

David W. Matula

Department of Computer Science
Southern Methodist University
Dallas, Texas 75275

April 1976

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Max Clique problem

- ER(N,p)   Random variable *X(N,p)*: Max Clique of ER(N,p)

$$Z(N,p) = 2log_{\frac{1}{p}}(N) - 2log_{\frac{1}{p}}\left(log_{\frac{1}{p}}(N)\right) + 2log_{\frac{1}{p}}\left(\frac{e}{2}\right) + 1$$

$$N \to \infty \qquad X(N,p) = \lfloor Z(N,p \rfloor \ or \ \lceil Z(N,p \rceil$$

- Good approximation for ER(N,1/2):

$$M_{max}(N) = 2log_2(N) - 2log_2\left(log_2(N)\right) + 2log_2\left(\frac{e}{2}\right) + 1$$

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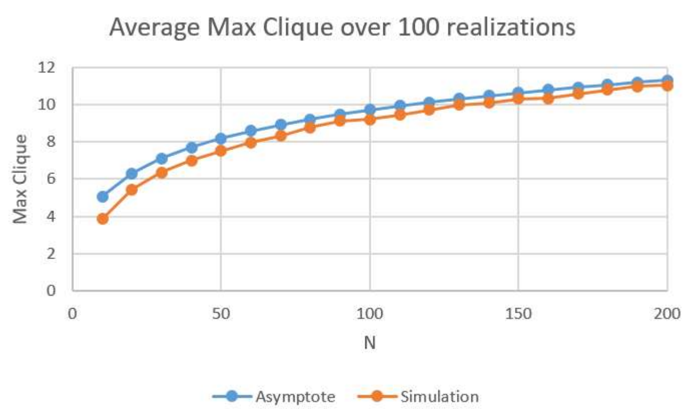
Max Clique problem

ER(N,1/2)



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Max Clique problem

M_{rand}

Math. Proc. Camb. Phil. Soc. (1975), **77**, 313
MPCPS 77–27
Printed in Great Britain

On colouring random graphs

BY G. R. GRIMMETT AND C. J. H. McDIARMID
Mathematical Institute, Oxford

$$M_{rand}(N) \sim log_{\frac{1}{p}}(N)$$

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Max Clique problem

Random algorithm:

```
Label the nodes
Clique = node 1

Loop
   Take next node
   Is node connected to all nodes in current clique?
      Yes? Add node to clique
```

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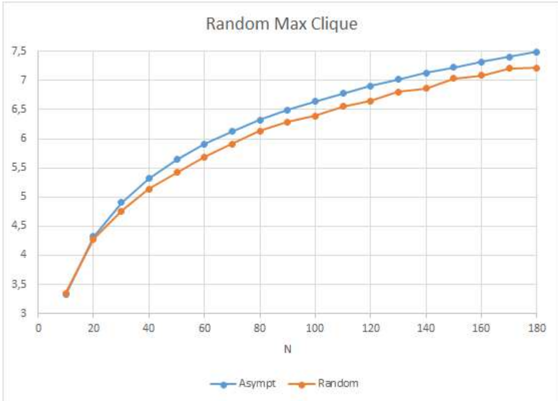
Max Clique problem



ER(N,1/2)

N = 180; M = 1000; T = 0.1 s

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Max Clique problem

```
 N =  100000
 M =  10
avg clique size =  16.6
asympt =  16.61
--- 0.37 seconds ---
```

```
 N =  1000000
 M =  2
avg clique size =  20.0
asympt =  19.93
--- 1.34 seconds ---
```


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Max Clique problem

arXiv > quant-ph > arXiv:2302.00639

Quantum Physics

[Submitted on 1 Feb 2023]

Q-score Max-Clique: The First Quantum Metric Evaluation on Multiple Computational Paradigms

Ward van der Schoot, Robert Wezeman, Niels M. P. Neumann, Frank Phillipson, Rob Kooij

TNO

Max Clique problem

Table 1: Q-scores Max-Clique with a 60 seconds time limit.

	Approach	Q-score
Classical	Tabu search	4,900
	Simulated annealing	9,100
Quantum Annealer	D-Wave Advantage	110
	D-Wave 2000Q	70
Hybrid ←	Hybrid solver	12,500
Gate-based	Starmon-5 (QAOA)	5*
	IBM-Guadalupe (QAOA)	$\geq 5*$

Max Clique problem

Table 1: Q-scores Max-Clique with a 60 seconds time limit.

	Approach	Simulated Q-score
Gate-based ←	QAOA	$\geq 16^*$
Photonics ←	Photonics	$\geq 20*$

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Other NP hard problems

frontiers in PHYSICS
REVIEW ARTICLE
published: 12 February 2014
doi: 10.3389/fphy.2014.00005

Ising formulations of many NP problems

*Andrew Lucas**
Lyman Laboratory of Physics, Department of Physics, Harvard University, Cambridge, MA, USA

https://blog.xa0.de/post/List-of-QUBO-formulations/#fn:V21

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List of QUBO formulations

Below a list of 112 optimization problems and a reference to the QUBO formulation of each problem is shown. While a lot of these problems are classical optimization problems from

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Other NP hard problems

- K - densest subgraph
- Minimum vertex covering
- Maximal matching
- Clique covering
- Number of perfect matchings
- Hamiltonian cycles
- Longest path
- Graph isomorphism
- …

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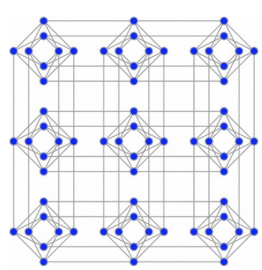
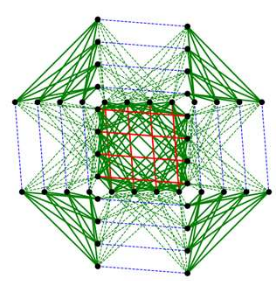
Other connections with Graph Theory

- D-WAVE QPU architectures



Chimera graph



Zephyr graph

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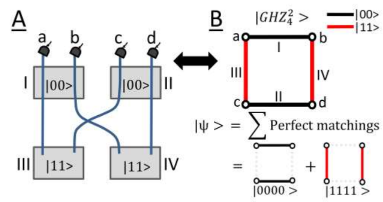
Other connections with Graph Theory

Quantum Experiments and Graphs III:
High-Dimensional and Multi-Particle Entanglement

Xuemei Gu,[1,2,*] Lijun Chen,[1,†] Anton Zeilinger,[2,3,‡] and Mario Krenn[2,3,§]

Graph Theory	Quantum Experiments
undirected Graph	optical setup with nonlinear crystals
Vertex	optical output path
Edge	nonlinear crystal
colors of the edge	mode numbers
perfect matching	n-fold coincidence
#(perfect matchings)	#(terms in quantum state)



- Greenberger-Horne-Zeilinger state $|\psi\rangle_{abcd} = \frac{1}{\sqrt{2}}(|0000\rangle + |1111\rangle)$

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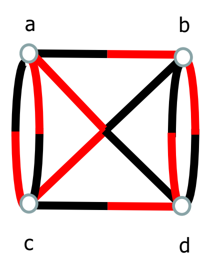
Other connections with Graph Theory

- Extension to Dicke states

$$|D_n^k\rangle = \frac{1}{\sqrt{\binom{n}{k}}}\hat{S}(|0\rangle^{\otimes(n-k)}|1\rangle^{\otimes k})$$

- Involves multi-graphs with multi-colored edges

- Found a new case of $|D_4^2\rangle$



$$|\Psi_{abcd} > \frac{1}{\sqrt{6}}(|0011\rangle + |0101\rangle + |0110\rangle + |1001\rangle + |1010\rangle + |1100\rangle)$$

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Wrap-up

- Graph Theory Inspired by Quantum Technology
- Asymptotic expressions for NP-hard problems
- Implementations on D-Wave
- Embeddings on D-Wave graphs
- Properties of multi-graphs with bi-colored edges

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