The Unreasonable Effectiveness of (Classical) Automated Reasoning in Quantum

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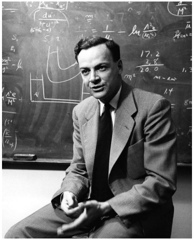
Quantum Computing

*"Nature isn't classical, d****t, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy."*



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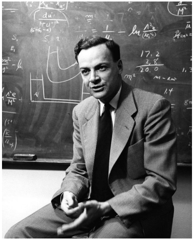

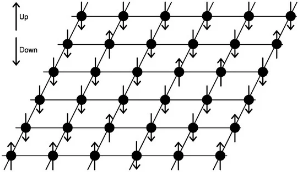

Computing spins requires exponentially many calculations

Quantum Computing

Feynman's conception: the quantum computer

- Turn the problem around: Let's make nature's complexity work for us

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Feynman's conception: the quantum computer

- Turn the problem around: Let's make nature's complexity work for us
- Progress: Google's [1] and IBM's [2] quantum supremacy experiments

[1] F. Arute, K. Arya, R. Babbush, D. Bacon, J. C. Bardin, et al., "Quantum supremacy using a programmable superconducting processor," *Nature*, vol. 574, 2019.

[2] Y. Kim, A. Eddins, S. Anand, K. X. Wei, E. Van Den Berg, et al., "Evidence for the utility of quantum computing before fault tolerance," *Nature*, vol. 618, 2023.

Quantum Computing Skepticism

Obstacles

- What if the (error-corrected) quantum computer never materializes?

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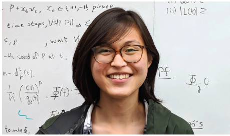
- What if it turns out that BQP $=$ P?



Ewin Tang [1] gave efficient classical algorithms for the recommender problem (at age 18)

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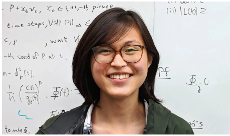

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Quantum computing Optimism

- There are (arguably) good arguments against this skepticism, but ...

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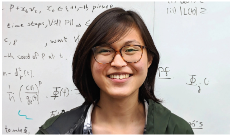

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- Nature keeps posing "quantum-hard" questions
  - Cracking problems in quantum computing solves quantum-hard problems
  - Applications in the simulation of physical systems, quantum chemistry, etc

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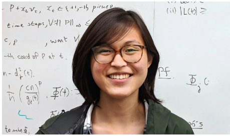

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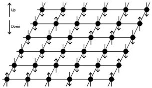
  - Applications in the simulation of physical systems, quantum chemistry, etc
- Our results with quantum circuits can be translated back to physics applications.



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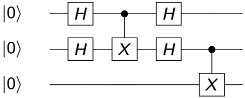

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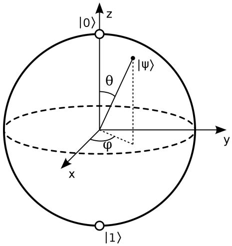
On the Road to Quantum Supremacy

How can we contribute?

- Build an (error-corrected) quantum computer
- Come up with a new quantum algorithm that shows that BQP $\neq P$



On the Road to Quantum Supremacy

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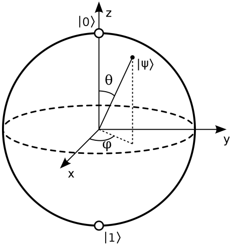
- Come up with a new quantum algorithm that shows that BQP $\neq P$
- Invent the tools to use current and future quantum computers



Quantum Circuit Compilation

Compilation is essential

- Efficiently utilize early frugale quantum computers
- Error correction requires hybrid solutions with fast classical components

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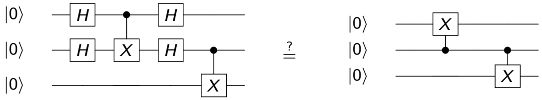
Compilation entails...

- Quantum circuit optimization



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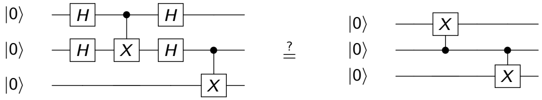
- Quantum circuit synthesis



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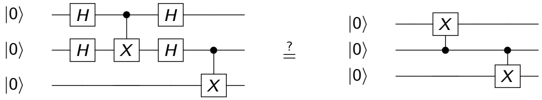
Compilation entails...

- Quantum circuit optimization
- Quantum circuit synthesis
- Quantum circuit simulation (a subtask in various analyses)



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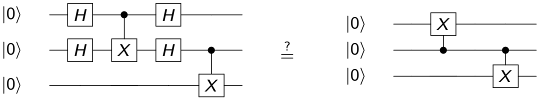
Compilation entails...

- Quantum circuit optimization
- Quantum circuit synthesis
- Quantum circuit simulation (a subtask in various analyses)
- Quantum circuit equivalence checking (for checking correctness)



Automated Reasoning in Quantum Circuit Compilation

Automated Reasoning Method

- Decision diagrams
- SAT / SMT / #SAT

$\times$

Quantum Circuit Compilation

- simulation
- equivalence checking
- optimization / synthesis

Automated Reasoning in Quantum Circuit Compilation

Automated Reasoning Method

- Decision diagrams
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×

Quantum Circuit Compilation

- simulation
- equivalence checking
- optimization / synthesis

(Translating results back Quantum Physics)

"Quantum computing becomes easy once you take the physics out of it"

Scott Aaronson

"Quantum computing becomes easy once you take the physics out of it"

Scott Aaronson

"Quantum computing becomes <u>even easier</u> once you take the <u>most linear algebra</u> out of it"

Alfons Laarman

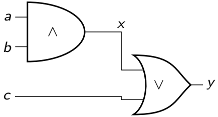
Quantum State

$$\vec{v} = \left.\begin{bmatrix} i \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \end{bmatrix}\right\} 2^n \text{ complex probability amplitudes}$$

Quantum State

$$\vec{V} = \begin{array}{r} \text{index } \overbrace{000\ldots000}^{\text{computational basis state}} : \\ \text{index } 000\ldots001 : \\ \text{index } 000\ldots010 : \\ \text{index } 000\ldots011 : \\ \vdots \\ \\ \\ \text{index } \underbrace{111\ldots111} : \end{array} \left.\begin{bmatrix} i \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \end{bmatrix}\right\} 2^n \text{ complex probability amplitudes}$$

Quantum Gate / Circuit



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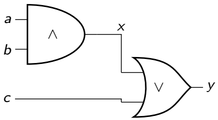

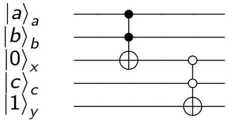

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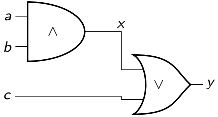

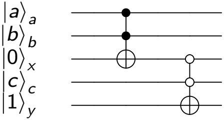

$$\underbrace{\begin{bmatrix} 1 & 0 & \dots & -i \\ \vdots & \vdots & \ddots & \vdots \\ i & 0 & \dots & 1 \end{bmatrix}}_{2^n} \left.\vphantom{\begin{bmatrix} 1 \\ \vdots \\ i \end{bmatrix}}\right\} 2^n$$

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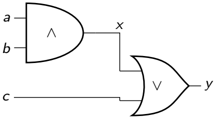

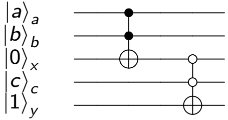

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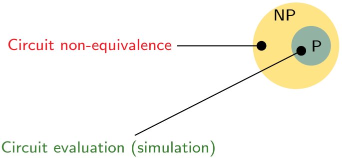
Simulation of quantum circuits: $G_k \cdots G_1 \cdot \vec{v}$

“Quantum P” and “Quantum NP”



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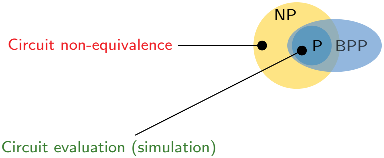

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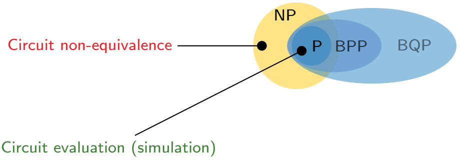

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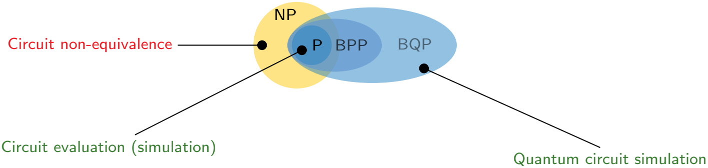

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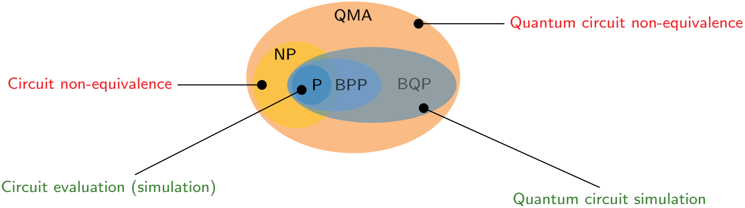

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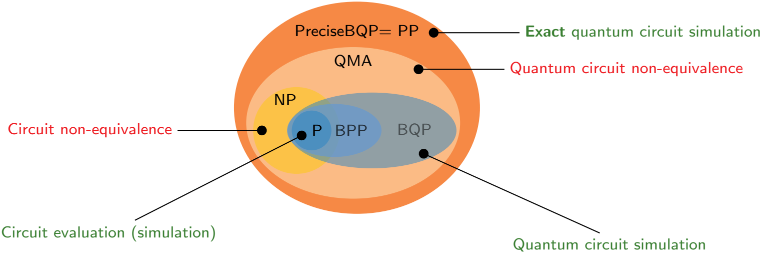

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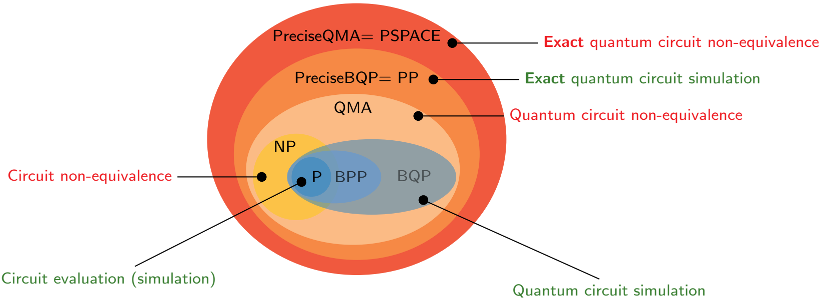

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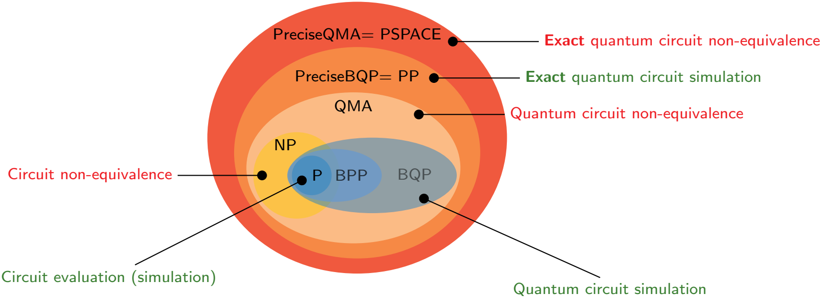

Despite hardness, we often focus on exact methods!

- This enables symbolic computation
- We can solve approximate problems using exact methods [1, 2].

[1] C.-Y. Wei, Y.-H. Tsai, C.-S. Jhang, and J.-H. R. Jiang, "Accurate BDD-based unitary operator manipulation for scalable and robust quantum circuit verification," in *Proceedings of the 59th ACM/IEEE Design Automation Conference*, 2022.

[2] X. Hong, M. Ying, Y. Feng, X. Zhou, and S. Li, "Approximate equivalence checking of noisy quantum circuits," in *2021 58th ACM/IEEE Design Automation Conference (DAC)*, 2021.

Satisfiability in Quantum Circuit Compilation

(A very incomplete overview)

SAT-based Quantum Circuit Simulation

✓ Efficient SAT encoding

✗ Non-universal

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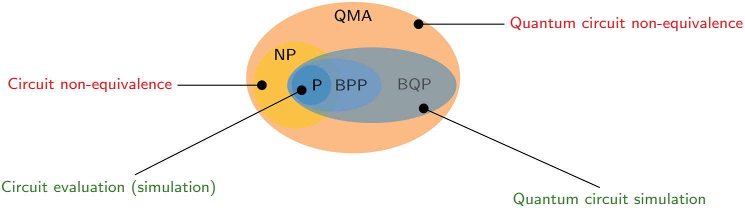
Berent et al. — Towards a SAT Encoding for .. [1]

- Stabilizer circuit simulation (non-universal)
- Stabilizer circuit equivalence checking (non-universal)



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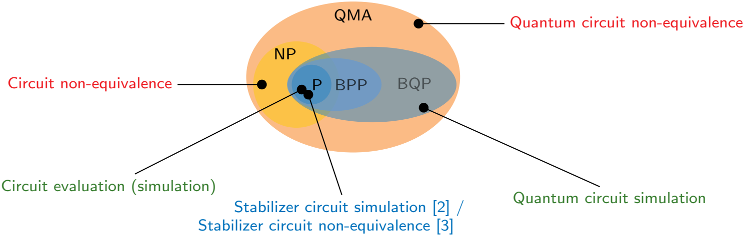

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symQV: Automated Symbolic Verification of ... [1]

- Efficient SMT-encoding of universal quantum circuits

$$\vec{v} = \begin{bmatrix} \sqrt{i} \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

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✗ Intractable SMT theory
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symQV: Automated Symbolic Verification of ... [1]

- Efficient SMT-encoding of universal quantum circuits
- Uses undecidable theory: NLA with trigonometric expressions
- Limited scaling

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Simulating Quantum Circuits by Weighted Model Counting (WMC)[1]

- Use density matrix instead of state vector

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- Negative weights: constructive and destructive interference

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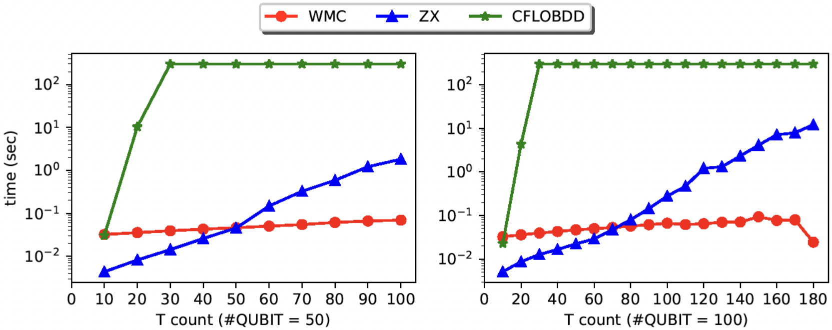

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#SAT-based Quantum Circuit Simulation

Equivalence Checking ... by Weighted Model Counting (WMC)[1]

- Use the same $\mathcal{O}(n+m)$ WMC encoding

[1] J. Mei, T. Coopmans, M. Bonsangue, and A. Laarman, "Equivalence checking of quantum circuits by model counting," in *IJCAR*, 2024.

[2] D. Thanos, T. Coopmans, and A. Laarman, "Fast equivalence checking of quantum circuits of Clifford gates," in *ATVA*, 2023.

#SAT-based Quantum Circuit Simulation

Equivalence Checking ... by Weighted Model Counting (WMC)[1]

- Use the same $\mathcal{O}(n + m)$ WMC encoding
- Combine with equivalence checking theorem from [2]

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Decision Diagrams in Quantum Circuit Compilation

Quantum State Representation with Decision Diagrams

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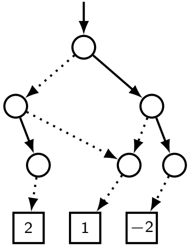

Multi-Terminal DD (MTBDD)

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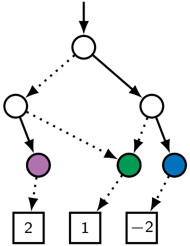

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$f_{00} = f_{10} = \begin{bmatrix} 1, \\ 0 \end{bmatrix}$

$f_{01} = \quad 2 \cdot f_{00}$

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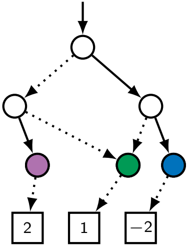

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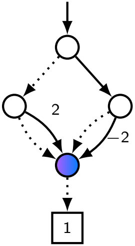

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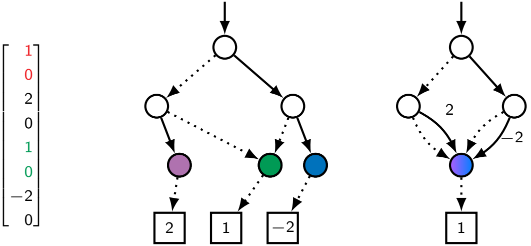

Multi-Terminal DD (MTBDD) Edge-Valued DD (EVDD)

Merge nodes v, w: $\vec{v} = \vec{w}$ $\vec{v} = \gamma \cdot \vec{w}$

(equivalent up to a complex factor λ)

(EVDD can be exponentially more succinct than MTBDD.)

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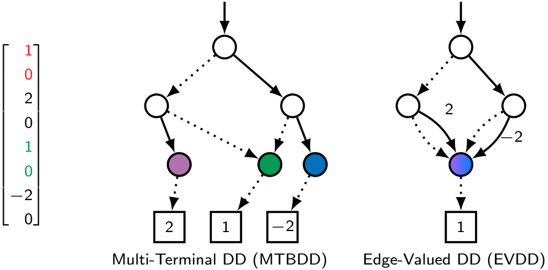

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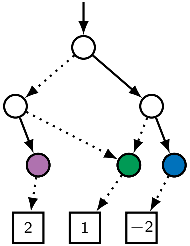

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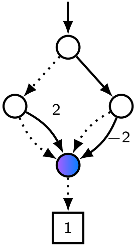

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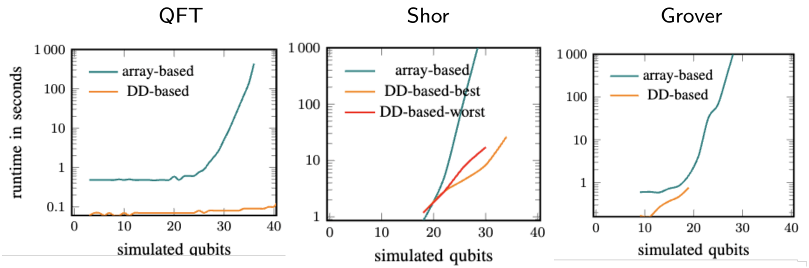
Performance of DD-based methods



Performance Characteristics for Simulation [1]

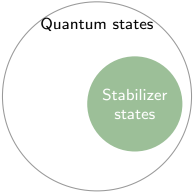
- Very fast and memory-efficient for structured quantum circuits
- EVDD is prone to numerical instability [2]; exact representations solve this [3]

[1] T. Grurl, J. Fuß, S. Hillmich, L. Burgholzer, and R. Wille, "Arrays vs. decision diagrams: A case study on quantum circuit simulators," in *ISMVL*, IEEE, 2020.

[2] P. Niemann, A. Zulehner, R. Drechsler, and R. Wille, "Overcoming the tradeoff between accuracy and compactness in decision diagrams for quantum computation," *CADICS*, vol. 39, 2020.

[3] Y.-H. Tsai, J.-H. R. Jiang, and C.-S. Jhang, "Bit-slicing the Hilbert space: Scaling up accurate quantum circuit simulation," in *2021 58th ACM/IEEE Design Automation Conference (DAC)*, 2021.

Analysis of Quantum Decision Diagrams



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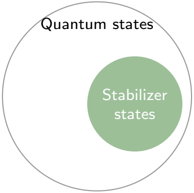

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EVDD can't succinctly represent stabilizer states, yet:

- Stabilizers are a subset of states that are classically simulatable!
- Important in error correction, measurement-based QC and circuit equivalence

Theorem ([1])

EVDD requires $2^{\Omega(n)}$ space to represent $n \times n$ grid graph states.

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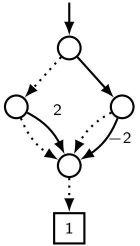
Local Invertible Map DD (LIMDD)



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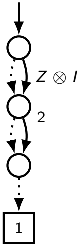

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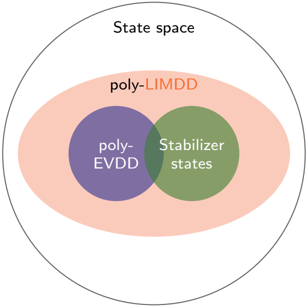

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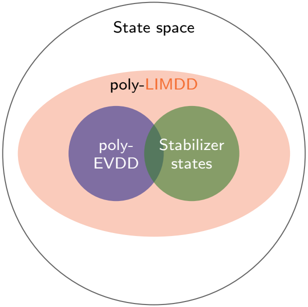
- Fidelity and inner product are not tractable [2]



	Queries					Manipulation operations						
	Sample	Measure	Equal	InnerProd	Fidelity	Addition	Hadamard	X,Y,Z	CZ	Swap	Local	T-gate
MTBDD	✓'	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
EVDD	✓'	✓	✓	✓	✓	✖	✖	✓	✓	✖	✖	✓
LIMDD	✓'	✓	✓	○	○	✖	✖	✓	✓	✖	✖	✓

✓ = tractable
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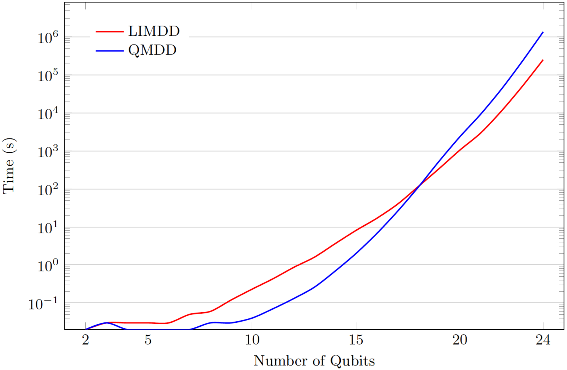
LIMDD Implementation

Circuit equivalence check implementation

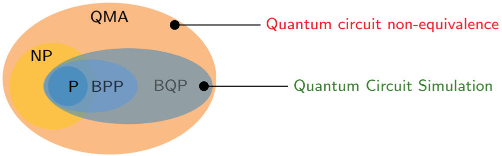
- LIMDD implemented in DDSIM [**limdd2**].
- Tested on QFT, after random Clifford circuit

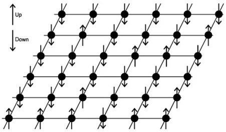


`https://github.com/cda-tum/mqt-limdd`

Concluding

Translating Back to Physics





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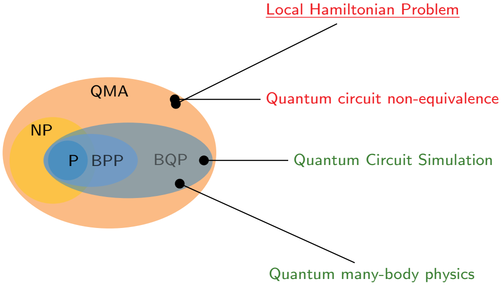
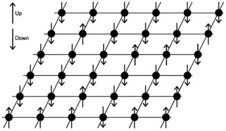
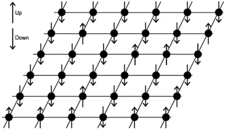




QMA-hard and BQP-hard Problems

- Finding the ground state / energy
- Computing the temperature of a system
- Quantum many-body physics

Translating Back to Physics



Physicists use tensor networks (e.g. **MPS**) and restricted Boltzmann Machines (**RBM**) to analyze these problems (in very similar ways to our use of DDs!)

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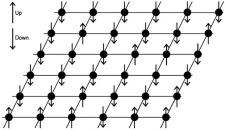

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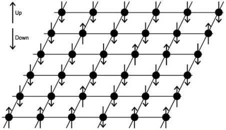

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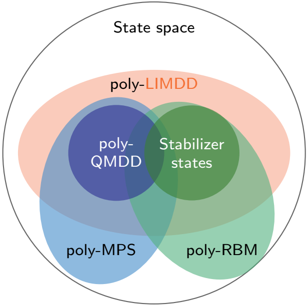

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