A study of QAOA using the Jülich Universal Quantum Computer Simulator

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Simulating quantum computers

N-qubit wave function:

$$|\psi\rangle = a_{0\cdots000}|0\cdots000\rangle + a_{0\cdots001}|0\cdots001\rangle + a_{0\cdots010}|0\cdots010\rangle + \cdots + a_{1\cdots111}|1\cdots111\rangle$$

$$= \left.\begin{pmatrix} a_{0\cdots000} \\ a_{0\cdots001} \\ a_{0\cdots010} \\ \vdots \\ a_{1\cdots111} \end{pmatrix}\right\} 2^N \text{ complex coefficients}$$

→ Storage requires (complex double precision)

$16 \times 2^N = 2^{N+4}$ B of RAM

$N = 4 \to$ 256B

$N = 16 \to$ 1MiB

$N = 31 \to$ 32GiB

$N = 42 \to$ 64TiB

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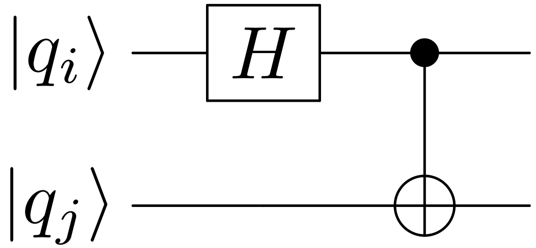
Simulating quantum computers



- Operations usually single- or two-qubit gates
  - → Update of the state vector in two- or four-component updates
  - → For single qubit gate U:

$$
\begin{aligned}
a_{***0***} &\leftarrow U_{00}a_{***0***} + U_{01}a_{***1***} \\
a_{***1***} &\leftarrow U_{10}a_{***0***} + U_{11}a_{***1***}
\end{aligned}
$$

The Jülich Universal Quantum Computer Simulator (JUQCS)

- JUQCS
  - → full state vector simulator (used for quantum supremacy)
  - → simulates an ideal gate-based quantum computer
  - → uses an efficient MPI communication scheme (distributed memory)
  - → runs on supercomputers
- How many qubits can we simulate?
  - → Qubit number limited by available RAM
  - → My Notebook: 30 qubits
  - → At JSC:

    43 qubits on Juwels Cluster/Booster

    42 qubits on Juwels Booster (GPUs) → much faster

Arute et al., Nature **574**, 505 (2019)

De Raedt et al., CPC **176**, 121 (2007)

De Raedt et al., CPC **237**, 47 (2019)

Willsch et al., arXiv:2104.03293 (2021)

The Quantum Approximate Optimization Algorithm (QAOA)

- Variational algorithm to find approximate solutions to optimization problems
- Variational state: $|\beta, \gamma\rangle = \prod_{k=1}^{p} \exp(-i\beta_k H_D) \exp(-i\gamma_k H_C) |+\rangle^{\otimes N}$

  where
  - β_k, γ_k variational parameters,
  - $H_D = \sum_{i=0}^{N-1} \sigma_i^x$ mixing Hamiltonian,
  - $H_C = \sum_{i=0}^{N-1} h_i \sigma_i^z + \sum_{i<j} J_{ij} \sigma_i^z \sigma_j^z$ problem Hamiltonian
- H_C encodes the optimization problem
- Optimize for $E_p^* = \min_{\beta,\gamma} \langle \beta, \gamma | H_C | \beta, \gamma \rangle$

Farhi et al., arXiv:1411.4028 (2014)

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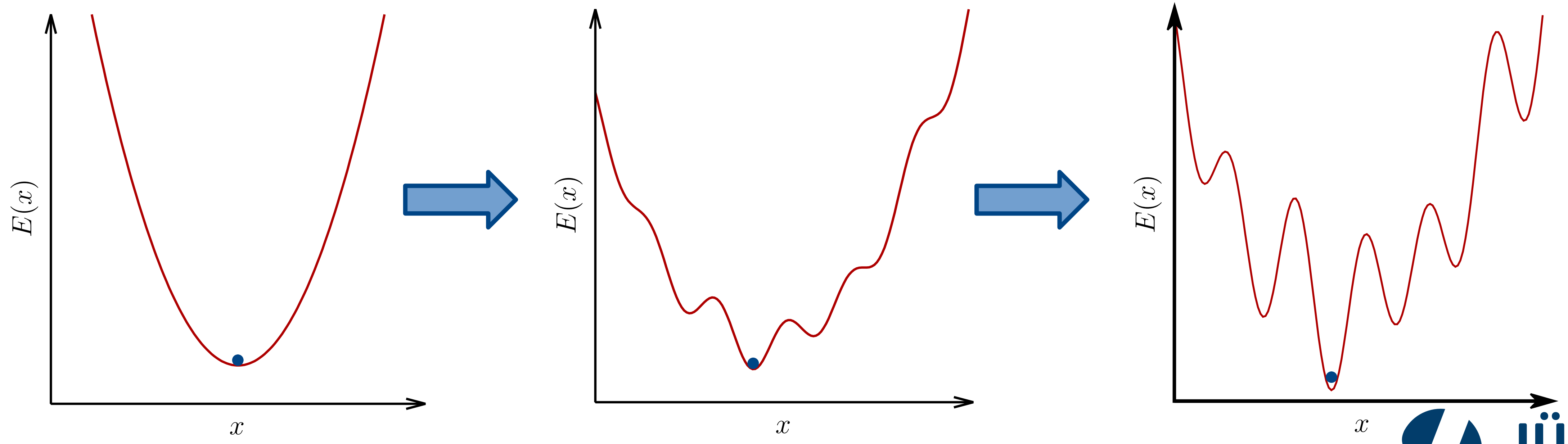
Relation between QAOA and quantum annealing

What is quantum annealing?

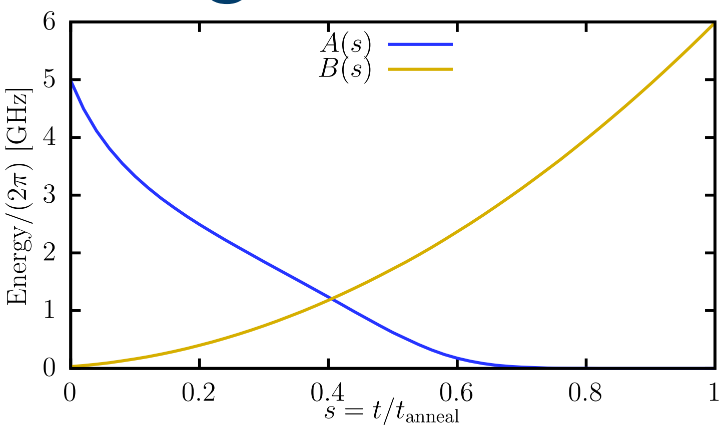
Idea based on adiabatic theorem:

- Quantum system initialized in ground state of Hamiltonian $H(t{=}0)$
- Hamiltonian $H(t)$ changes (sufficiently slowly) with time

➔ Quantum system stays in instantaneous eigenstate



Relation between QAOA and quantum annealing



annealing schedule

- Quantum annealing Hamiltonian

$$H(s) = A(s)H_{\mathrm{init}} + B(s)H_{\mathrm{final}}, \quad s = t/t_{\mathrm{anneal}}$$

where

$$A(0) \gg B(0) \approx 0, \quad B(1) \gg A(1) \approx 0.$$

$$H_{\mathrm{init}} = -\sum_{i=0}^{N-1} \sigma_i^x$$

$$H_{\mathrm{final}} = \sum_{i=0}^{N-1} h_i \sigma_i^z + \sum_{i<j} J_{ij} \sigma_i^z \sigma_j^z$$

Familiar from QAOA's H_D and H_C

- Simulate time evolution of quantum system (solve TDSE) under the Hamiltonian $H(s)$ with Suzuki-Trotter product-formula algorithm De Raedt, Comp. Phys. Rep. **7**, 1 (1987)

  → Decomposition looks like a QAOA variational state

Willsch et al., QIP **19**, 197 (2020)

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Relation between QAOA and quantum annealing

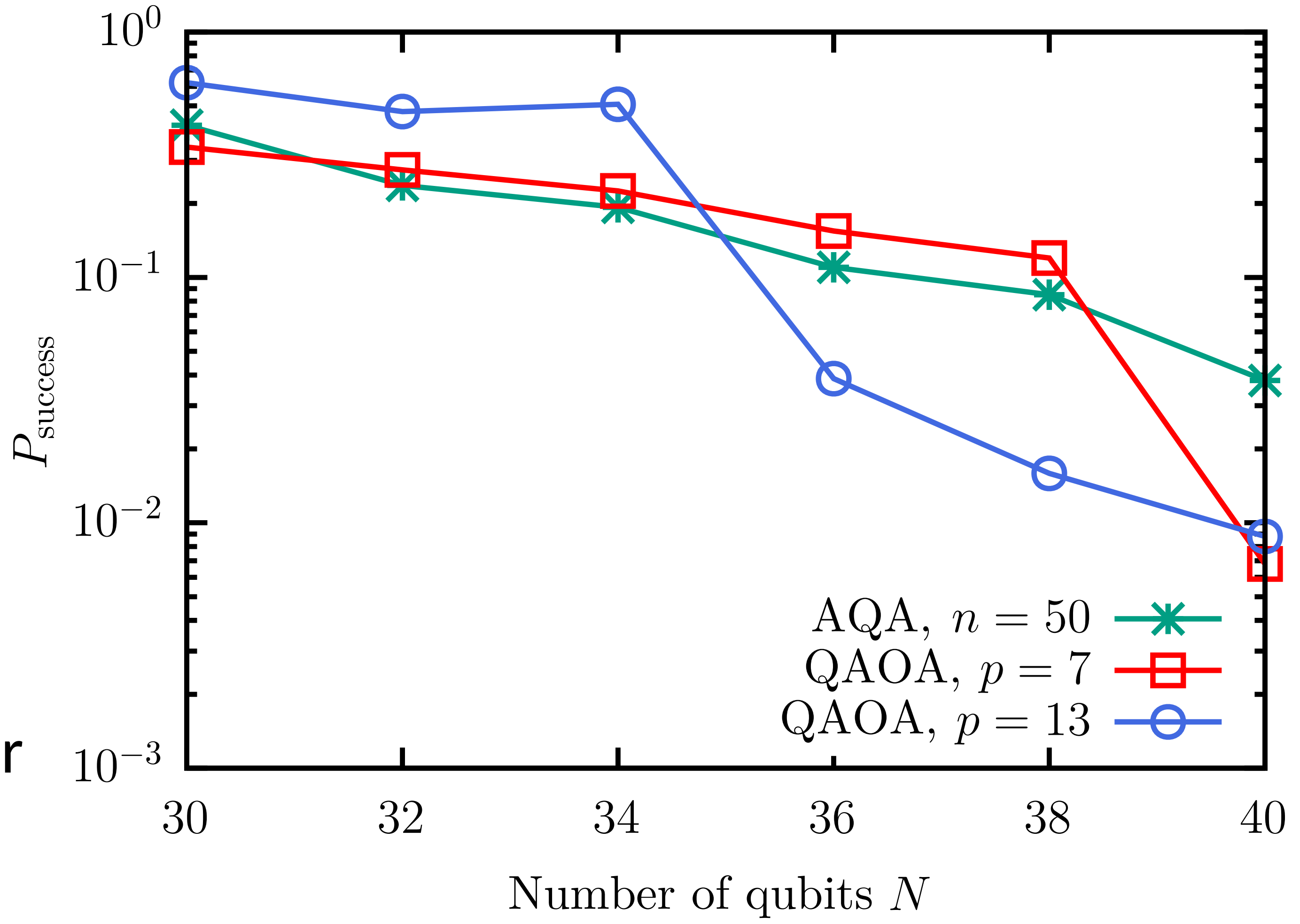
Approximate Quantum Annealing (AQA)

- Product-formula of quantum annealing
  - Coarse discretization with large time step
    → Not accurate enough for genuine QA
  - and a small number of steps
    → Time too short for adiabatic evolution
- AQA as an independent, heuristic method
- AQA as initialization for variational parameters of QAOA
- We use exact cover problems with 30-40 qubits in our study

Willsch et al.,
arXiv:2104.03293 (2021)

Results: QAOA and AQA performance

- Similar success probabilities with AQA and QAOA
  - → Where probability drops for QAOA, optimizer probably got stuck in local minimum
- For AQA, number of steps 50, for QAOA much smaller
  - → BUT QAOA required of the order of 150-200 JUQCS calls/energy evaluations for optimization



Willsch et al., arXiv:2104.03293 (2021)

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Efficiency of QAOA and AQA

- AQA with p steps requires same run time as single energy evaluation for p-step QAOA
  - → This QAOA evaluation does not include the optimization
  - → If optimization requires m energy evaluations, p-step QAOA runs m times as long as p-step AQA
  - → In the same time it takes for p-step QAOA, we can run $m \times p$-step AQA
  - → p-step QAOA as efficient as n-step AQA if $m \leq n/p$ energy evaluations needed
- Does AQA solve all the problems?
  - → Probably not, as we do not expect $m \times p$-step AQA to work very well on current NISQ devices

Willsch et al., arXiv:2104.03293 (2021)

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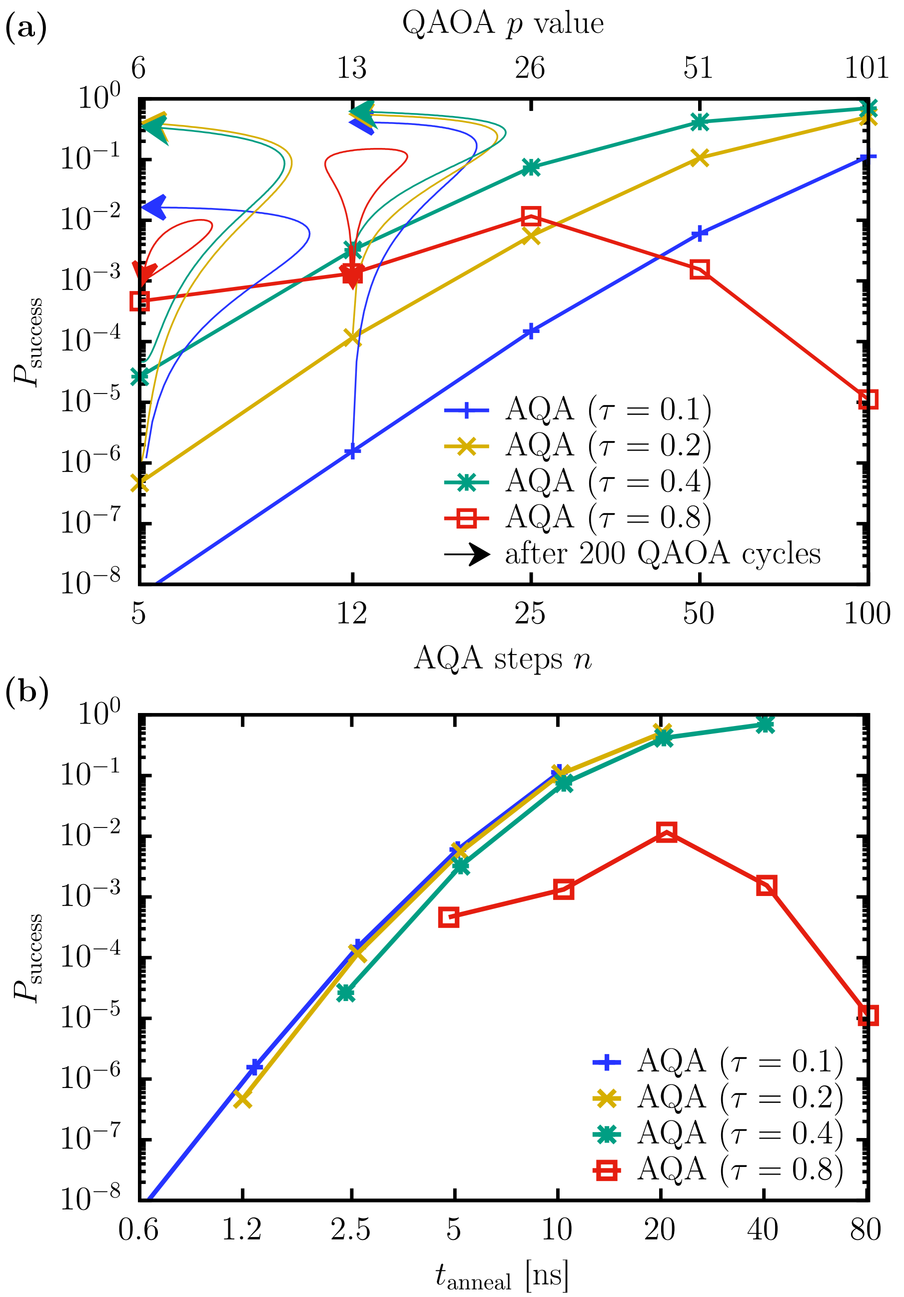
Results: AQA as initialization for QAOA

Standalone AQA vs. AQA as initialization for QAOA

- Standalone AQA
  - → Success probability increases with number of steps (if $\tau \leq 0.4$ ns)
  - → Success probability increases with step size τ up to $\tau = 0.4$ ns

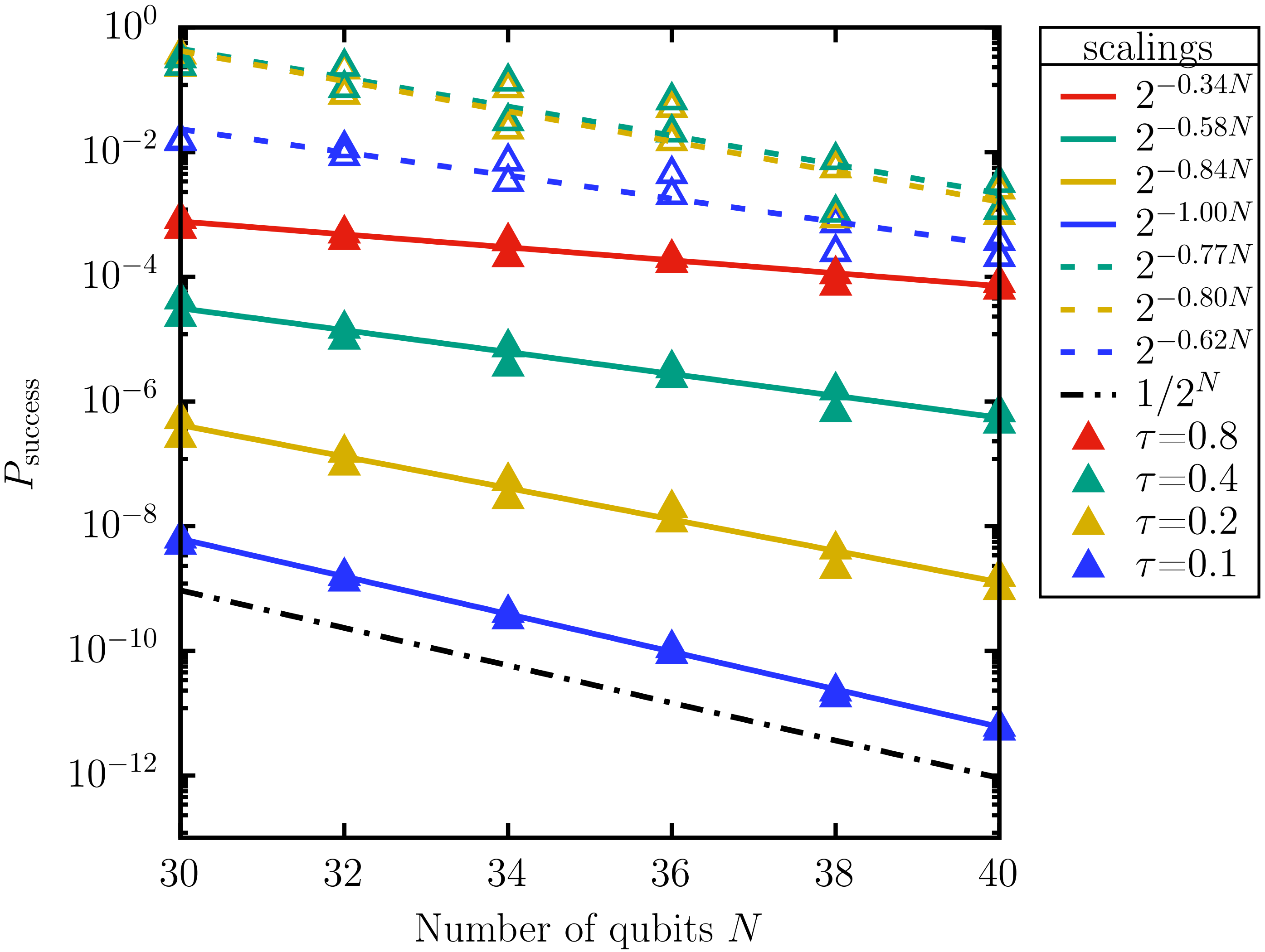
- QAOA with AQA-initialization
  - → Improved success probabilities for $\tau \leq 0.4$ ns
  - → For $\tau = 0.8$ ns no visible improvement

- For large number of steps AQA better, for small number of steps QAOA better



Results: QAOA and AQA scalings

- QAOA (dashed lines)
  - → Parameters optimized for a 30-qubit instance
  - → For all other instances the same parameters are used
  - → Success probabilities quite large
  - → Scaling with qubit number exponential
- AQA (solid lines)
  - → Scaling also exponential but with smaller prefactor in exponent for larger step size τ



Willsch et al., arXiv:2104.03293 (2021)

Summary and outlook

- Introduction of
  - → JUQCS
  - → QAOA
  - → Quantum annealing
  - → AQA
- Comparison of QAOA and AQA
  - → Performance
  - → Efficiency
  - → Scaling

- Outlook
  - → Simulation results look promising
  - → Future steps: Test of AQA on genuine quantum hardware with ≥ 30 qubits, several hundreds of gates
  - → Also test on different problem sets

D. Willsch, M. Willsch, F. Jin,
K. Michielsen and H. De Raedt,
arXiv:2104.03293 (2021)

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Thank you for your attention