

# Quantum algorithm design for many- body simulation



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# Institute for Quantum Information RWTH Aachen

- Our focus areas:
  - A. Mathematical foundations of quantum information
  - B. Quantum algorithm development
- Cluster of Excellence: Matter and Light for Quantum Computing (ML4Q )
- Visiting Reader at Department of Computing Imperial College London
- Industry ties, e.g., with Amazon Web Services Center for Quantum Computing

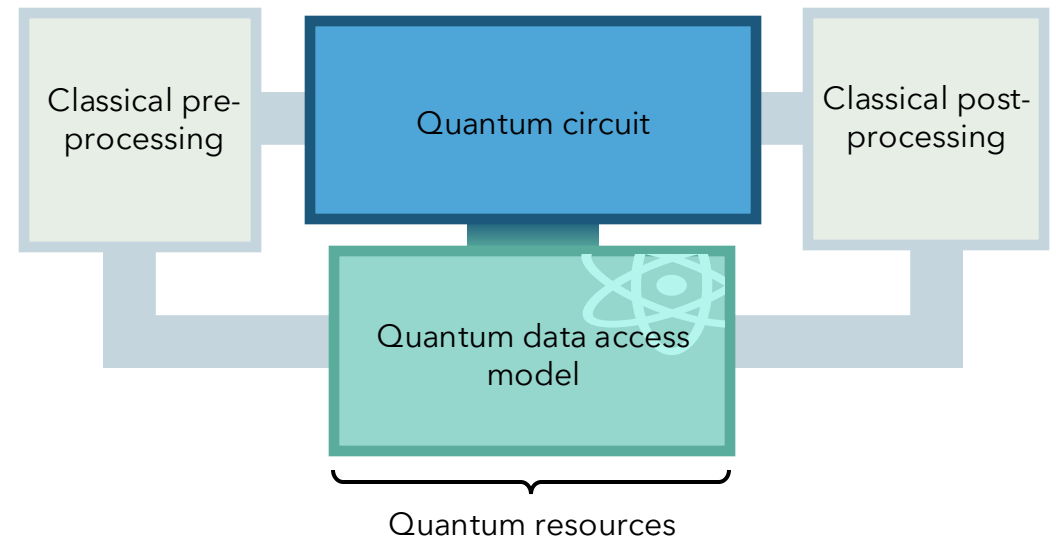


# Quantum algorithm development

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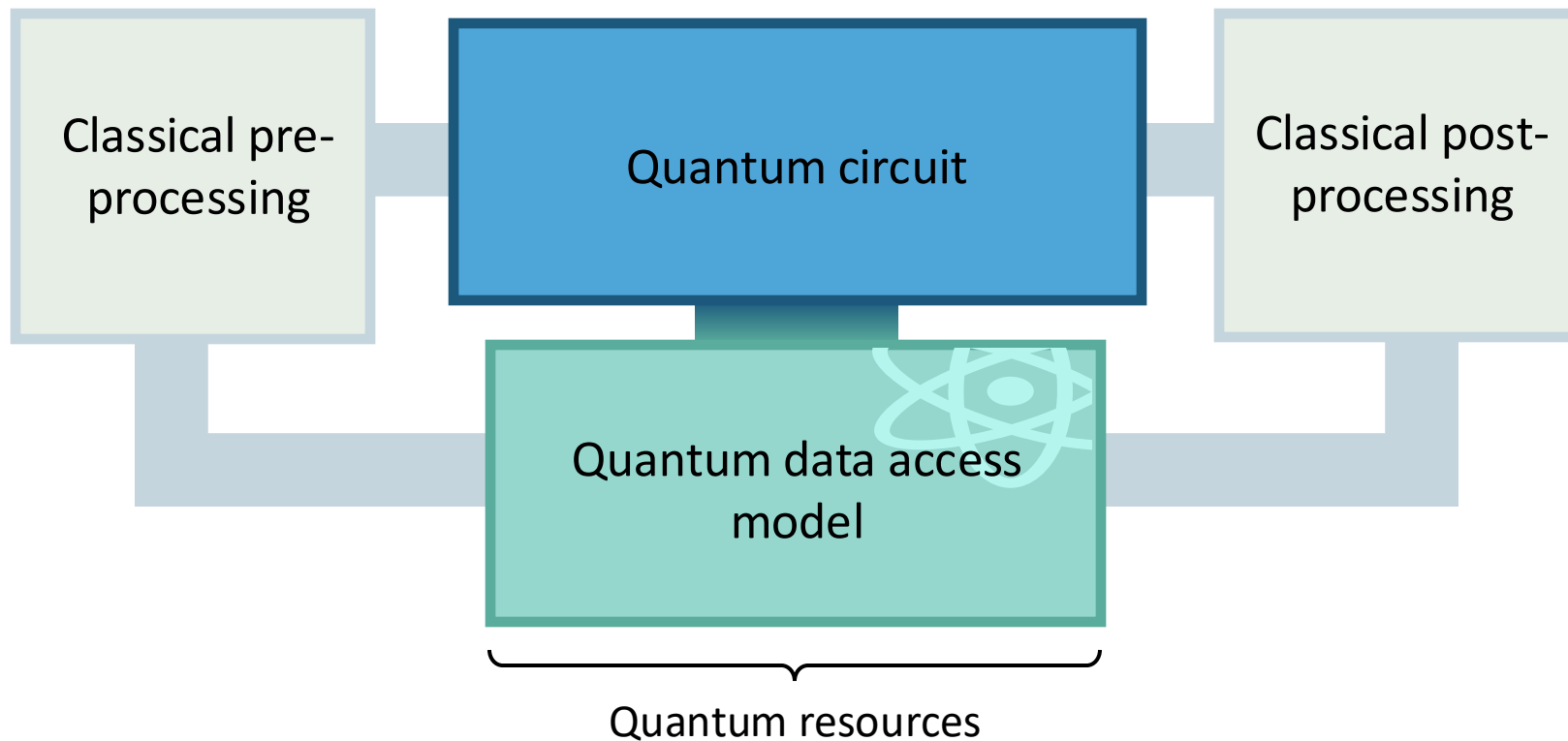
# Classical versus quantum technologies

- *Do algorithms based on **quantum components**, including*
  - *quantum processing units (QPU)*
  - *quantum random access memory (QRAM)**provide **computational advantages** compared to classical components?*
- Goal is to identify use cases / areas of applications with
  - large (super-quadratic) quantum speed-up
  - minimal quantum footprint, i.e., use classical routines whenever possible
  - no galactic algorithms



# Early fault-tolerant quantum algorithms

- Hybrid classical-quantum schemes with end-to-end complexity analysis



- Complexity estimates for comparison with [state-of-the-art classical methods](#)

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# Quantum algorithms:

A survey of applications and end-to-end complexities

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Quantum  
Algorithms  
Wiki

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# Quantum Algorithms Wiki

## PART I AREAS OF APPLICATION

### Condensed matter physics

- 1.1 Fermi–Hubbard model
- 1.2 Spin models
- 1.3 SYK model

### Quantum chemistry

- 2.1 Simulating electrons in molecules and materials
- 2.2 Simulating vibrations in molecules and materials

### Nuclear and particle physics

- 3.1 Quantum field theories
- 3.2 Nuclear physics

### Combinatorial optimization

- 4.1 Search algorithms à la Grover
- 4.2 Beyond quadratic speedups in exact combinatorial optimization

### Continuous optimization

- 5.1 Zero-sum games: Computing Nash equilibria
- 5.2 Conic programming: Solving LPs, SOCPs, and SDPs
- 5.3 General convex optimization
- 5.4 Nonconvex optimization: Escaping saddle points and finding local minima

### Cryptanalysis

- 6.1 Breaking cryptosystems
- 6.2 Weakening cryptosystems

### Solving differential equations

### Finance

- 8.1 Portfolio optimization
- 8.2 Monte Carlo methods: Option pricing

### Machine learning with classical data

- 9.1 Quantum machine learning via quantum linear algebra
- 9.2 Quantum machine learning via energy-based models
- 9.3 Tensor PCA
- 9.4 Topological data analysis
- 9.5 Quantum neural networks and quantum kernel methods

## PART II QUANTUM ALGORITHMIC PRIMITIVES

### Quantum linear algebra

- 10.1 Block-encodings
- 10.2 Manipulating block-encodings
- 10.3 Quantum signal processing
- 10.4 Qubitization
- 10.5 Quantum singular value transformation

### Hamiltonian simulation

- 11.1 Product formulas
- 11.2 qDRIFT
- 11.3 Taylor and Dyson series (linear combination of unitaries)
- 11.4 Quantum signal processing / quantum singular value transformation

### Quantum Fourier transform

### Quantum phase estimation

### Amplitude amplification and estimation

- 14.1 Amplitude amplification
- 14.2 Amplitude estimation

### Gibbs sampling

### Quantum adiabatic algorithm

### Loading classical data

- 17.1 Quantum random access memory
- 17.2 Preparing quantum states from classical data
- 17.3 Block-encoding dense matrices of classical data

### Quantum linear system solvers

### Quantum gradient estimation

### Variational quantum algorithms

### Quantum tomography

### Quantum interior point methods

### Multiplicative weights update method

### Approximate tensor network contraction

## PART III FAULT-TOLERANT QUANTUM COMPUTING

### Basics of fault tolerance

### Quantum error correction with the surface code

### Logical gates with the surface code

| Appendix | Background, conventions, and notation   |
|----------|-----------------------------------------|
| A.1      | Quantum systems and bra-ket notation    |
| A.2      | The quantum circuit model               |
| A.3      | Noise in quantum gates and the NISQ era |
| A.4      | Big- $O$ notation                       |
| A.5      | Complexity theory background            |

### References

### Index

# Ground states via Quantum phase estimation

## **Randomized quantum algorithm for statistical phase estimation**

Physical Review Letters (2022) with Campbell & Wan

Quantum Information Processing (QIP) 2022

## **Qubit-efficient randomized quantum algorithms for linear algebra**

PRX Quantum (2024) with McArdle & Wang

Quantum Computing Theory in Practice (QCTiP) 2023

Theory of Quantum Computation, Communication and Cryptography (TQC) 2023

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# Thermal states via Quantum Gibbs samplers

## **Polynomial time quantum Gibbs sampling for Fermi-Hubbard model at any temperature**

Nature Communications, conditionally accepted (2025) with Šmíd, Meister, and Bondesan

Quantum Computing Theory in Practice (QCTiP) 2025

Theory of Quantum Computation, Communication and Cryptography (TQC) 2025

## **Rapid mixing of quantum Gibbs samplers for weakly-interacting quantum systems**

arXiv:2510.04954 (2025) with Šmíd, Meister, and Bondesan

# Quantum Gibbs samplers

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# Question: Gibbs state preparation

- Goal: Given  $n$ -qubit Hamiltonian  $H$  and inverse temperature  $\beta = T^{-1} > 0$ , prepare the quantum Gibbs states  $\sigma_\beta = \frac{\exp(-\beta H)}{Z}$  with  $Z = \text{Tr}[\exp(-\beta H)]$  the partition function
- More precisely: Prepare up to precision  $\epsilon \in [0,1]$  in trace distance  $\|\cdot\|_{\text{Tr}}$  the purified Gibbs state

$$|\sqrt{\sigma_\beta}\rangle := Z^{-1/2} \sum_i \exp\left(-\frac{\beta E_i}{2}\right) |E_i\rangle \otimes |\bar{E}_i\rangle$$

- End-to-end extension: Compute the partition function  $Z$  up to relative error  $\epsilon \in [0,1]$
- Physical quantity: Estimate Helmholtz free energy  $F = -\beta^{-1} \log(Z)$  for different  $\beta > 0$
- Intuition: Classically exponentially difficult, polynomial heuristics can suffer, e.g., from the sign problem

# Example: Fermi-Hubbard model

- Hamiltonian on  $D$ -dimensional lattice given by

$$H_{FH} := -t \sum_{\langle i,j \rangle} \sum_{\sigma \in \{\uparrow, \downarrow\}} (a_{i,\sigma}^\dagger a_{j,\sigma} + a_{j,\sigma}^\dagger a_{i,\sigma}) + U \sum_i a_{i,\uparrow}^\dagger a_{i,\uparrow} a_{i,\downarrow}^\dagger a_{i,\downarrow}$$

- Applications, e.g., for Mott metal-insulator transition or high temperature superconductivity
- Can be hard for classical methods (for  $D \geq 2$ ) with unknown parts in phase diagram, e.g., the strange metal phase
- Standard computational benchmark
- Amenable to quantum methods in contrast to glassy spin systems? [Ansuetz *et al.*, QIP (2025)]

# Quantum approach(es)

- More quantum versions of Markov chain Monte Carlo [Temme *et al.*, Nature (2011)]  
→ delicate, partially missing rigorous guarantees, missing mixing time bounds
- Quantum singular value transformation [Gilyén *et al.*, STOC (2019)] → a priori exponentially expensive
- Lindbladian thermalization as **fully quantum version of Markov chain Monte Carlo**:
  - Exact **quantum detailed balance** AND step wise **algorithmic efficiency** [Chen *et al.*, QIP (2024)]
  - Quantum Glauber and Metropolis dynamics [Ding *et al.*, CMP (2025)] [Gilyén *et al.*, arXiv (2024)]
- Need bound on mixing time  $t_{\text{mix}} \cong$  number of steps:

|                     |                  |                        |
|---------------------|------------------|------------------------|
| $\text{polylog}(n)$ | $\text{poly}(n)$ | $\exp(\text{poly}(n))$ |
| rapid               | fast             | slow                   |



Chi-Fang (Anthony) Chen

# Simulated Lindbladian thermalization

- From  $\rho_0$  simulate dynamics  $\rho(t) = \exp(t\mathcal{L}^\dagger)[\rho_0]$  via Linbladian [Ding et al., CMP (2025)]

$$\mathcal{L}^\dagger[\rho] := -i[G, \rho] + \sum_{a \in \mathcal{A}} \left( L_a \rho L_a^\dagger - \frac{1}{2} \{L_a^\dagger L_a, \rho\} \right)$$

via the set  $\mathcal{A}$  of jump operators  $A^a$  and filter functions  $f^a(t)$  with

$$L_a := \int_{-\infty}^{\infty} f^a(t) \cdot \exp(itH) A^a \exp(-itH) dt$$

$$G := \sum_{a \in \mathcal{A}} \int_{-\infty}^{\infty} g(t) \cdot \exp(itH) (L_a^\dagger L_a) \exp(-iHt) dt \text{ for specific } g(t)$$

- Exact quantum detailed balance  $\mathcal{L}^\dagger[\sigma_\beta] = 0$  AND step wise algorithmic efficiency – via modern Hamiltonian simulation + coherent function preparation [McArdle, Gilyén, B., arXiv (2022)]

# Task: Bound mixing time

polylog(n)    poly(n)    exp(poly(n))  
 rapid                  fast                  slow

- Mixing time  $t_{\text{mix}}(\epsilon) := \inf \left\{ t \geq 0 : \left\| \exp(t\mathcal{L}^\dagger)[\rho_0] - \sigma_\beta \right\|_{\text{Tr}} \leq \epsilon \ \forall \rho_0 \right\}$

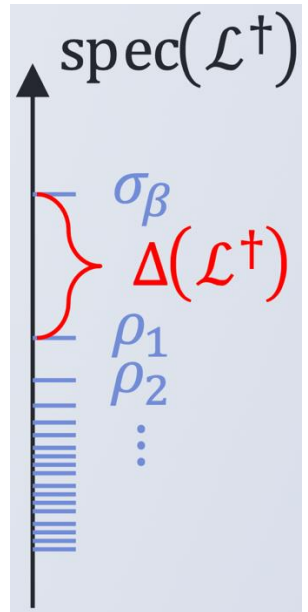
- Hölder gives spectral gap bound

$$t_{\text{mix}}(\epsilon) \leq \Delta(\mathcal{L}^\dagger)^{-1} \cdot \log \left( 2\epsilon^{-1} \left\| \sigma_\beta^{-1/2} \right\| \right) = \Delta(\mathcal{L}^\dagger)^{-1} \cdot O(n + \log(\epsilon^{-1}))$$

- Lindbladian is non-Hermitian, vectorization on doubled Hilbert space gives parent Hamiltonian via similarity transform

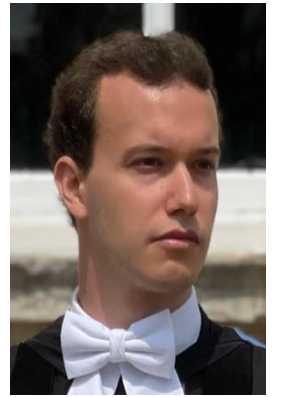
$$\mathcal{H}[\cdot] := \sigma_\beta^{-1/4} \mathcal{L}^\dagger \left[ \sigma_\beta^{1/4} (\cdot) \sigma_\beta^{1/4} \right] \sigma_\beta^{-1/4} \Rightarrow t_{\text{mix}}(\epsilon) \leq \Delta(\mathcal{H})^{-1} \cdot O(n + \log(\epsilon^{-1}))$$

- Understood, e.g., for high temperatures [Rouzé *et al.*, QIP (2024)]



# Theorem: Gibbs state preparation

- **Main result:** For any quasi-local fermionic Hamiltonian  $H = H_0 + \lambda \cdot V$  at any inverse temperature  $\beta > 0$ , there exists system size independent positive constants  $\lambda_{\max}, d$  such that for any  $|\lambda| \leq \lambda_{\max}$  the Lindbladian has spectral gap  $\Delta \geq \Delta_0 - d|\lambda|$ .
- **Corollary:** For  $H_0$  gapped and  $\lambda$  small enough, prepare purified Gibbs state in quantum complexity  $\tilde{O}(n^3 \cdot \text{polylog}(\epsilon^{-1}))$  and compute the partition function in quantum complexity  $\tilde{O}(n^5 \cdot \epsilon^{-2})$  using  $\tilde{O}(n)$  qubits.
  - rigorous polynomial end-to-end complexity versus, e.g., quantum phase estimation, no (rigorous) classical analogue!
  - NB: perturbative proof technique extends to other systems (e.g., Heisenberg model)



Štěpán Šmíd



# Proof: Free fermions

- Quadratic Hamiltonian  $H_0 = \sum_{i,j} \omega_i h_{ij} \omega_j = \boldsymbol{\omega}^T \cdot h \cdot \boldsymbol{\omega}$  with  $\omega_i$  Majorana fermion:  
 $\omega_i^\dagger = \omega_i$  and  $\{\omega_i, \omega_j\} = 2\delta_{ij} \rightarrow$  **exactly solvable Lindbladian  $\mathcal{L}_0$**
- Design choice:  $A^a = \omega_a$  Majorana jumps and  $\hat{f}^a = \hat{f} \forall a$  Gaussian for  $\mathcal{L}_0 \Rightarrow$  coherent term  $G = 0$
- Third quantization for vectorizing fermionic Lindbladians [Prosen, NJP (2008)]: Parent Hamiltonian  
 $\mathcal{H}_0 \cong -\boldsymbol{c}^\dagger \cdot S \cdot \boldsymbol{c} + \boldsymbol{c} \cdot S \cdot \boldsymbol{c}^\dagger + \boldsymbol{c}^\dagger \cdot A \cdot \boldsymbol{c}^\dagger + \boldsymbol{c} \cdot A \cdot \boldsymbol{c}$  for  $\{c_i^\dagger, c_i\}_{i=1}^{2n}$  and  $S, A$  simple functions of  $h$
- **System size independent gap  $\Delta(\mathcal{H}_0) \equiv \Delta_0 = 2 \cdot \exp(-4\beta^2 ||h||) \cosh(2\beta ||h||)$**
- NB: Free fermions even have rapid mixing  $t_{\text{mix}}^{[0]}(\epsilon) \leq \frac{1}{2\Delta_0} \log\left(\frac{\tanh(2\beta ||h||)}{2} \cdot \frac{n}{\epsilon}\right) = O(\text{polylog}(n))$

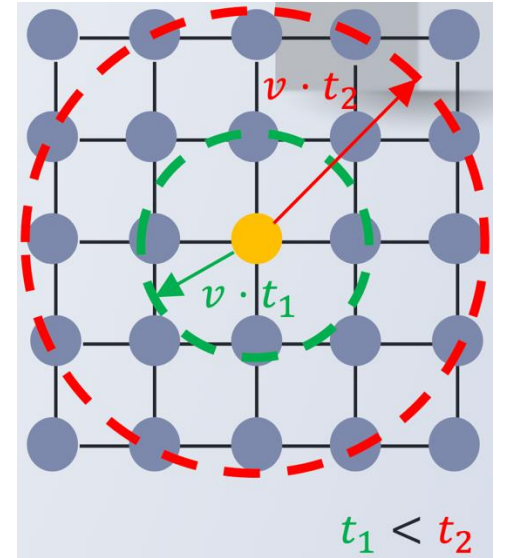
[Rapid mixing of quantum Gibbs samplers for weakly-interacting quantum systems, arXiv:2510.04954]

# Proof: Stability theorem

- **Tool:** Stability of spectral gap of free fermionic Hamiltonians under perturbation

[Hastings, J. Math. Phys. (2019)]  $\Rightarrow$  gap closes at most linearly in perturbation

- **Task:** Lift properties from fermionic Hamiltonian  $H = H_0 + \lambda \cdot V$  to parent Hamiltonian  $\mathcal{H} := \mathcal{H}_0 + \mathcal{V}$  of Lindbladian  $\Rightarrow$  study perturbation  $\mathcal{V}$



- **Proof steps:** (1) quasi-locality of perturbation  $\mathcal{V}$  (2) bounded strength of perturbation  $\mathcal{V}$  in  $\lambda$

- (1) Lieb-Robinson bounds [Haah et al., FOCS (2018)] on  $\tilde{L}_a := \exp(\beta H/4) L_a \exp(-\beta H/4)$  to

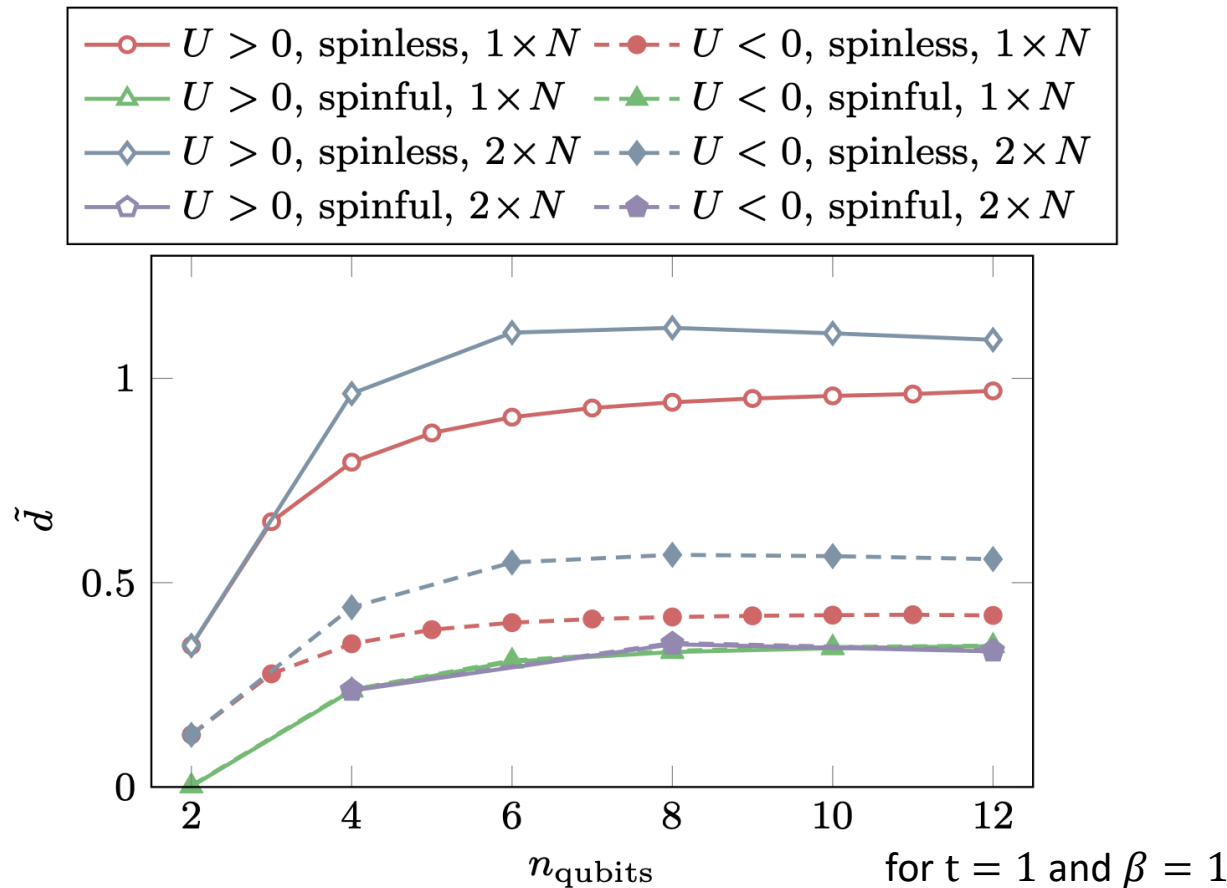
estimate  $\left\| \tilde{L}_a - \tilde{L}_a^{(r)} \right\| \leq c \cdot \exp(-\mu r)$  (and  $G_a$  terms in coherent part  $G$ )

(2) Duhamel's formula as  $\exp((A + B)t) = \exp(A) + \int_0^t \exp((A + B)(t - s)) \cdot B \cdot \exp(As) ds$  to

estimate  $\left\| \tilde{L}_a - \tilde{L}_a^0 \right\| \leq c \cdot |\lambda|$  (and  $G_a$  terms in coherent part  $G$ )

# Benchmark: Fermi-Hubbard weak coupling

- $U/t$  small with Majorana jump operators and Gaussian filter functions (analytical results)



- Slope of gap closing:

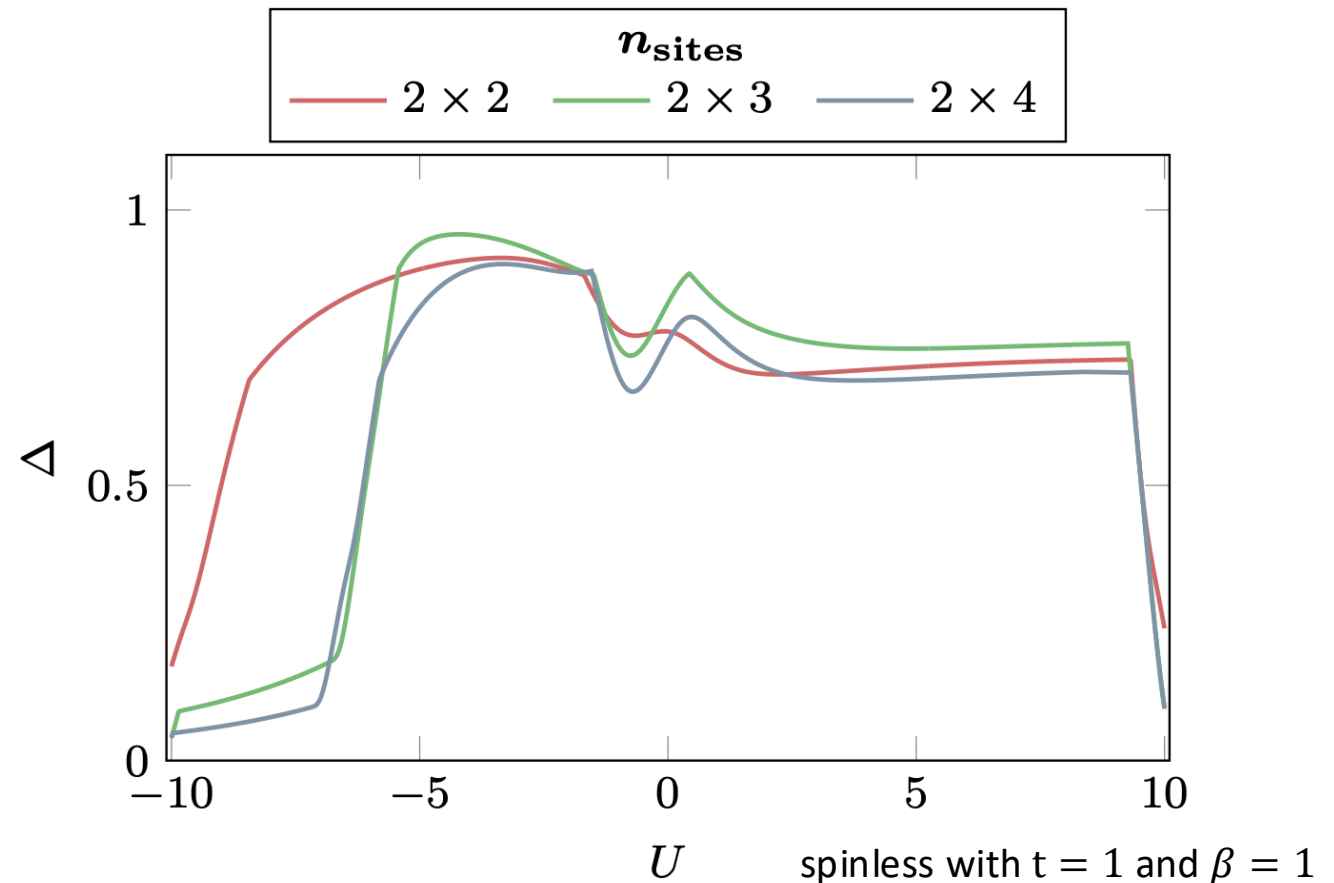
$$\tilde{d}^{\pm} := \mp \frac{\partial \Delta(\mathcal{L}^{\dagger})}{\partial U} \Big|_{U=0^{\pm}}$$

$\Rightarrow$  uniform upper bound in  $n$

- NB: Dependence  $\Delta_0 \sim \exp(-\beta^2)$   
beyond analytics much improved with
  - single site Pauli jump operators
  - Metropolis style filter functions

# Benchmark: Fermi-Hubbard medium coupling

- Intermediate  $2 \lesssim U/t \lesssim 6$  for  $D = 2$  with single site Pauli jump operators and Metropolis filter functions:
- NB: Again, favorable  $\beta \gg 1$  dependence with this design choice
- No analytics, need larger system sizes, e.g., for interplay of coupling strength and support of filter functions?





# Conclusion



# Summary

- **Main result:** Sampling properties of quantum Gibbs states in [end-to-end polynomial time quantum complexity](#) – in stark contrast to algorithms based on quantum phase estimation
- **Example end-to-end complexity:** Compute the partition function with  $\tilde{O}(n^5 \cdot \epsilon^{-2})$  quantum gates on  $\tilde{O}(n)$  qubits for (weakly) interacting Fermi-Hubbard model
- **Extensions:**
  - Starting from  $t = 0$  atomic limit, [similar results for spinful  \$U/t \gg 1\$  strong coupling regime of Fermi-Hubbard model](#)
  - Other systems via perturbative gap techniques, e.g., Bose-Hubbard model, Heisenberg model, etc.
- **New:** Rapid mixing via oscillator norm techniques – overall, shaves off polynomial complexity factors  
[\[Rapid mixing of quantum Gibbs samplers for weakly-interacting quantum systems, arXiv:2510.04954\]](#)

# Outlook

- Larger scale numerical simulations (e.g., tensor network based) – versus leading classical heuristics  
– versus analogue quantum simulators?
- Faster (heuristic) algorithms all the way down to (quasi-) linear  $\tilde{O}(n \cdot \text{polylog}(\epsilon^{-1}))$ , via rapid mixing and adaptive jump operators?
- Improved effective mixing time for specific (local) information?
- More tools to develop around quantum Gibbs samplers:
  - Verify convergence (heuristically) without a priori guarantees
  - Make noise tolerance quantitative
  - Applications in optimization theory



Extra material





SCHWERPUNKT

QUANTENCOMPUTING

# Algorithmen für neue Hardware

Quantenalgorithmen lösen nur bestimmte Rechenprobleme signifikant effizienter als klassische Algorithmen.

Mario Berta

- Guiding questions:
  - What quantum algorithms do we eventually want to run?
  - For what applications is the quantum footprint the smallest to become competitive with classical methods?
- 50-100 error corrected qubits could allow for meaningful tests
- That's it, thank you

