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

European Research Council

MATTER AND LIGHT FOR QUANTUM COMPUTING

Imperial College London

EPSRC

aws

Bundesministerium für Bildung und Forschung

quanten technologien

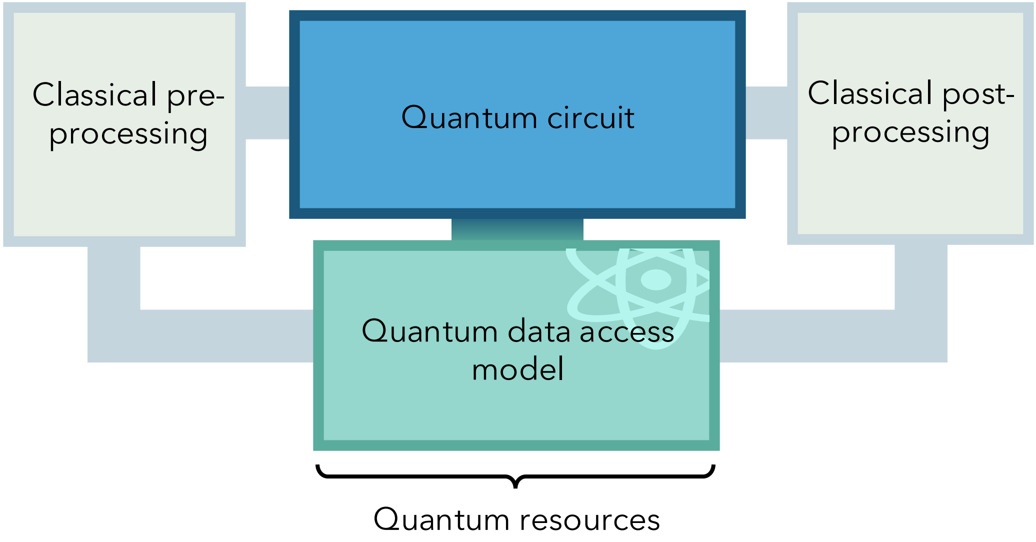
Quantum algorithm development

Classical versus quantum technologies

- *Do algorithms based on quantum components, including*
  - *quantum processing units (QPU)*
  - *quantum random access memory (QRAM)*

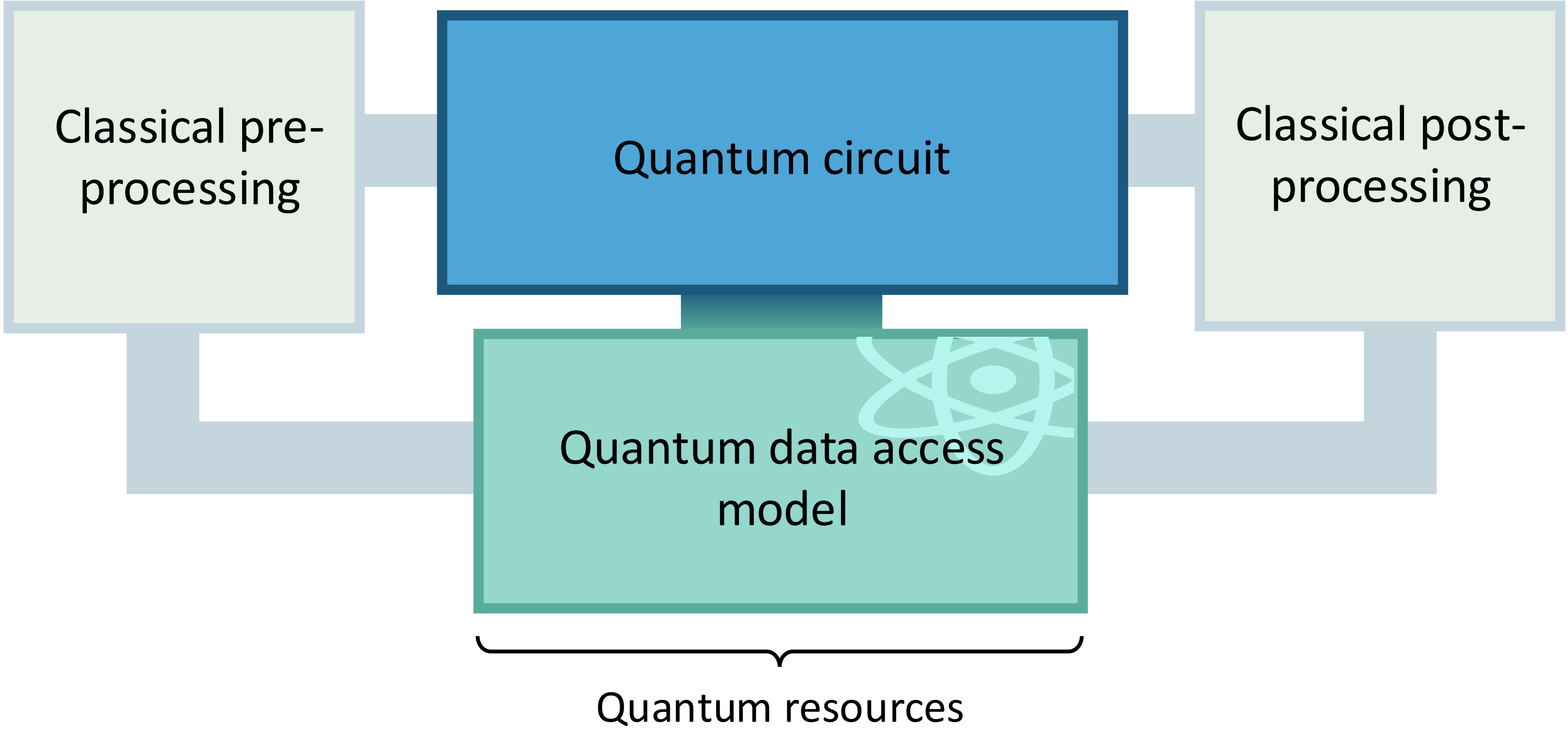
provide computational advantages compared to classical components?

- 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

Quantum algorithms:

A survey of applications and end-to-end complexities

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Quantum Algorithms Wiki

Cambridge University Press
(2025)

[open access
arXiv:2310.03011]

Quantum Algorithms Wiki

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

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

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 $Z = \mathrm{Tr}[\exp(-\beta H)]$ the partition function
- More precisely: Prepare up to precision $\epsilon \in [0,1]$ in trace distance $\|\cdot\|_{\mathrm{Tr}}$ the purified Gibbs state

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

- 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

$$H_{FH} \coloneqq -t \sum_{<i,j>} \sum_{\sigma \in \{\uparrow,\downarrow\}} \left(a_{i,\sigma}^{\dagger} a_{j,\sigma} + a_{j,\sigma}^{\dagger} a_{i,\sigma}\right) + U \sum_{i} a_{i,\uparrow}^{\dagger} a_{i,\uparrow} a_{i,\downarrow}^{\dagger} a_{i,\downarrow}$$

- 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? [Anschuetz *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_{mix} ≅ number of steps:

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

Chi-Fang (Anthony) Chen

Simulated Lindbladian thermalization

- From ρ_0 simulate dynamics $\rho(t) = \exp\left(t\mathcal{L}^\dagger\right)[\rho_0]$ via Linbladian [Ding et al., CMP (2025)]

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

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

$$L_a \coloneqq \int_{-\infty}^{\infty} f^a(t)\cdot\exp(itH)A^a\exp(-itH)\mathrm{d}t$$

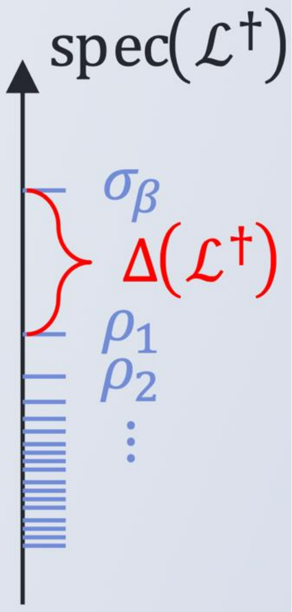
$$G \coloneqq \sum_{a\in\mathcal{A}}\int_{-\infty}^{\infty} g(t)\cdot\exp(itH)\left(L_a^\dagger L_a\right)\exp(-iHt)\mathrm{d}t \text{ for specific } g(t)$$

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

Task: Bound mixing time

$\mathrm{polylog}(n)$	$\mathrm{poly}(n)$	$\exp(\mathrm{poly}(n))$
rapid	fast	slow

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



- Hölder gives spectral gap bound

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

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

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

- 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 λ small enough, prepare purified Gibbs state in quantum complexity $\tilde{O}\left(n^3 \cdot \mathrm{polylog}(\epsilon^{-1})\right)$ 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)

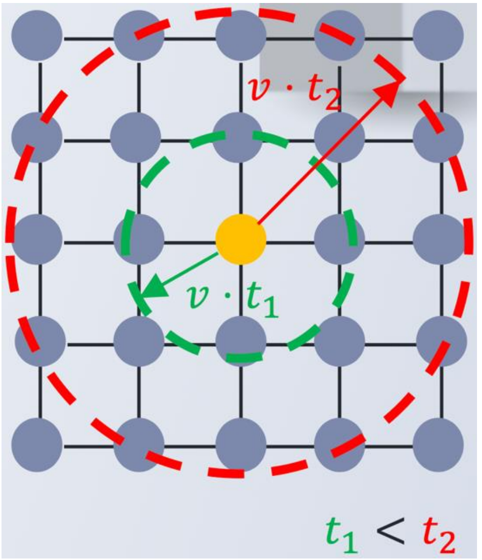
Štěpán Šmíd

Proof: Free fermions

- Quadratic Hamiltonian $H_0 = \sum_{i,j} \omega_i h_{ij} \omega_j = \boldsymbol{\omega}^{\boldsymbol{T}} \cdot h \cdot \boldsymbol{\omega}$ with ω_i Majorana fermion: $\omega_i^\dagger = \omega_i$ and $\{\omega_i, \omega_j\} = 2\delta_{ij}$ → 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 $t_{\mathrm{mix}}^{[0]}(\epsilon) \leq \frac{1}{2\Delta_0} \log\left(\frac{\tanh(2\beta||h||)}{2} \cdot \frac{n}{\epsilon}\right) = O\big(\mathrm{polylog}(n)\big)$

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

Proof: Stability theorem

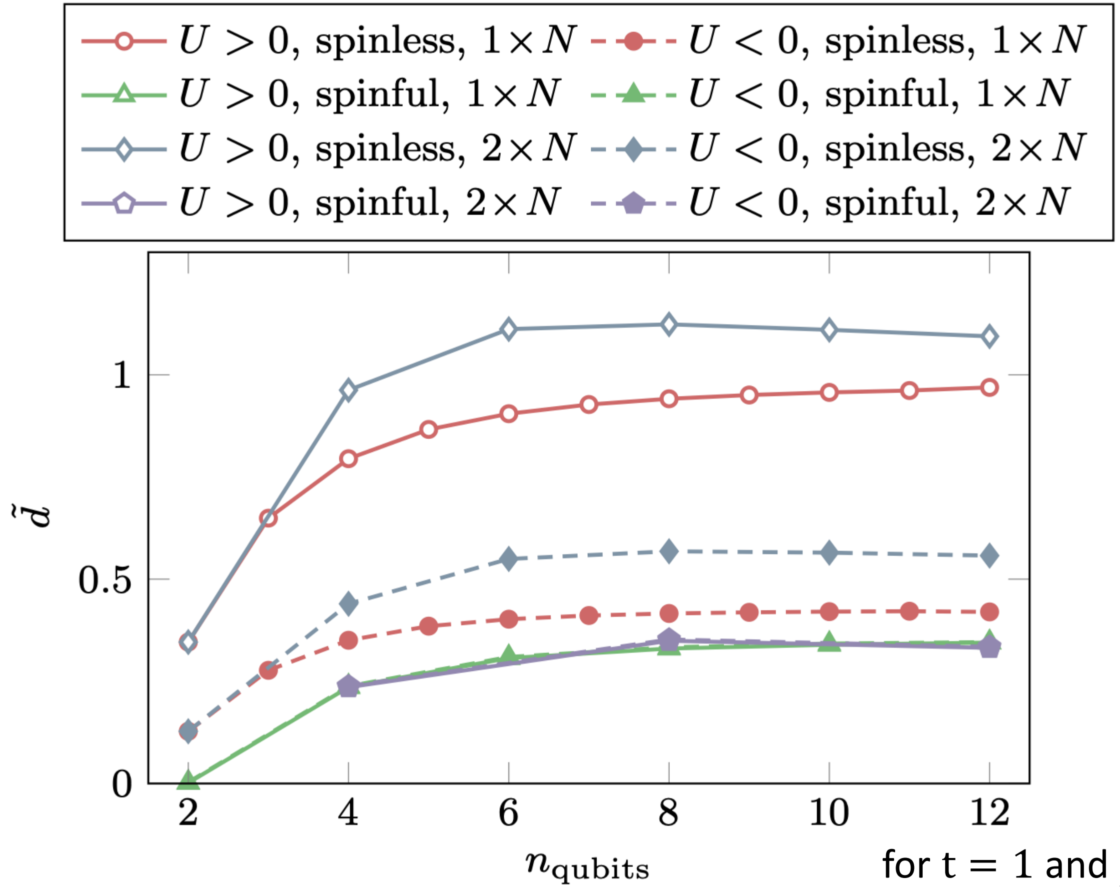


- **Tool**: Stability of spectral gap of free fermionic Hamiltonians under perturbation [Hastings, J. Math. Phys. (2019)] $\Rightarrow$ gap closes at most linearly in perturbation
- **Task**: Lift properties from fermionic Hamiltonian $H = H_0 + \lambda \cdot V$ to parent Hamiltonian $\mathcal{H} := \mathcal{H}_0 + \mathcal{V}$ of Lindbladian $\Rightarrow$ study perturbation $\mathcal{V}$
- **Proof steps**: (1) quasi-locality of perturbation $\mathcal{V}$ (2) bounded strength of perturbation $\mathcal{V}$ in λ
- (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 $\exp\big((A+B)t\big) = \exp(A) + \int_0^t \exp\big((A+B)(t-s)\big) \cdot B \cdot \exp(As) \mathrm{d}s$ 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)



for $t = 1$ and $\beta = 1$

- Slope of gap closing:

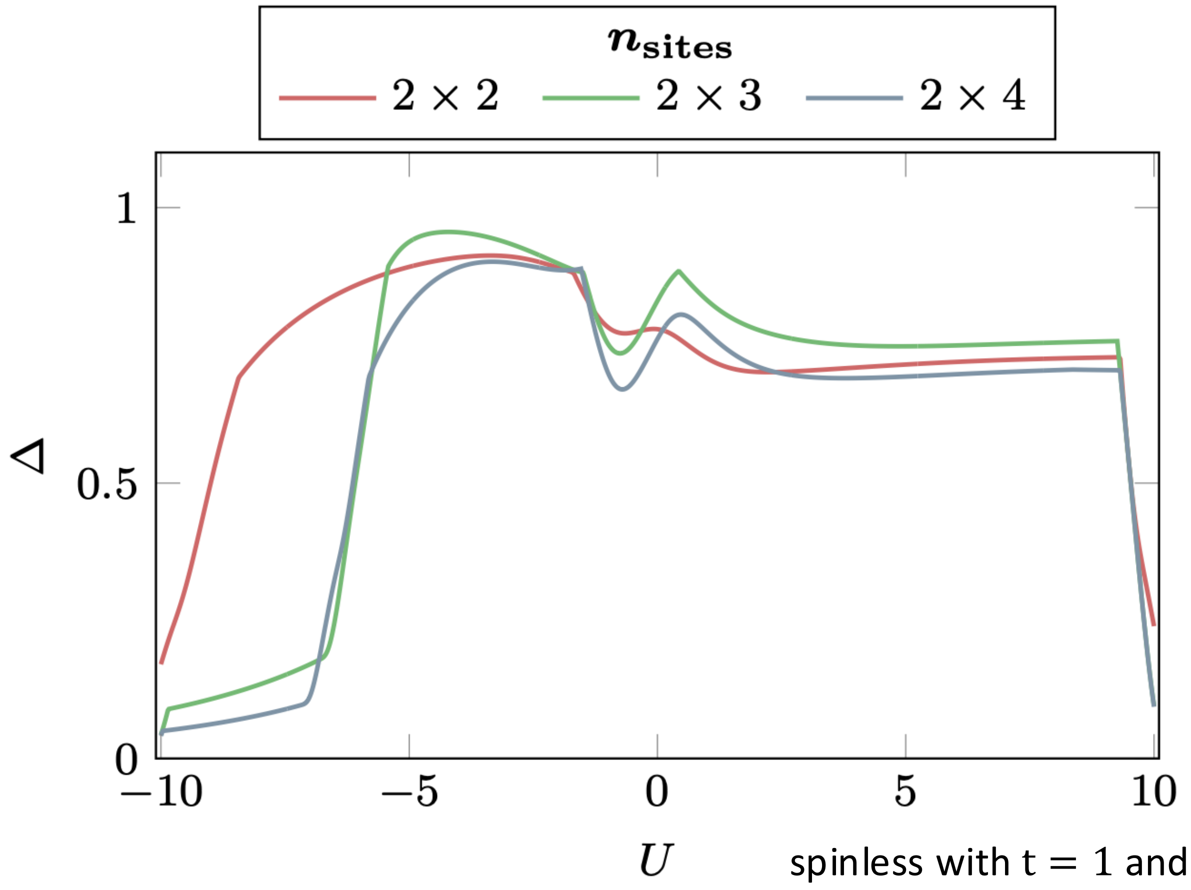
$$\tilde{d}^{\pm} := \mp \frac{\partial \Delta(\mathcal{L}^{\dagger})}{\partial U}\Big|_{U=0^{\pm}}$$

$\Rightarrow$ 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?



spinless with $\mathrm{t} = 1$ and $\beta = 1$

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 $\widetilde{\mathrm{O}}\left(n \cdot \mathrm{polylog}(\epsilon^{-1})\right)$, 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

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