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Discussion of stoquastic Hamiltonians

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Introduction

- Hamiltonian $H = \sum_i H_i$ is stoquastic if in some local basis $\mathcal{B}$ the terms H_i all have matrix entries that are zero or negative,

$$\langle x|H|y\rangle \leq 0 \quad , \quad \forall x, y \in \mathcal{B} \text{ with } x \neq y.$$

- H "doesn't have a sign problem", and its equilibrium states are on the border of quantum and classical complexity.

- Why should we care about these seemingly classical models with a basis dependent property?

- Because stoquastic H are fundamental in nature, and using classical tools to understand them is a miracle within QM.

Outline

- Central properties and examples
  - Perron-Frobenius theorem
  - Euclidean time path integrals
  - Example: spinless particles
  - Example: transverse Ising model
  - Impossibility of 'solving the sign problem'

- Complexity results and classical simulations
  - Stoquastic adiabatic computation
  - Ground state energy: prover and classical verifier
  - Excited states and time evolution
  - Monte Carlo methods
  - Rigorous results: ferromagnets and 1D
  - Frustration-free stoquastic AQC
  - Simulated quantum annealing

Part 1: central properties and examples

Perron Frobenius theorem: amplitudes in equilibrium

- If H has all real and non-positive matrix entries, then $A = -\beta H$ is a non-negative matrix. Expand e^A as a series,

$$e^A = 1 + A + \frac{A^2}{2} + ...$$

- Every term in the series is a nonnegative matrix, therefore $e^{-\beta H}$ is a nonnegative matrix.

- Since $\lim_{\beta\to\infty} e^{-\beta H} = |\psi\rangle\langle\psi|$, there is a choice of global phase which gives the ground state nonnegative amplitudes.

- If H is an irreducible matrix, then all of the ground state amplitudes are positive, $\psi(x) > 0$ for all $x \in \mathcal{B}$. (no nodes)

Euclidean time path integrals

- We can expand the partition function as a "path integral",

$$Z = \mathrm{tr}\left(e^{-\beta H}\right) = \sum_{x \in \mathcal{B}} \langle x| \left(e^{-\frac{\beta H}{L}}\right)^L |x\rangle = \sum_{x_1,\ldots,x_L \in \mathcal{B}} \prod_{i=1}^{L} \langle x_i| e^{-\frac{\beta H}{L}} |x_{i+1}\rangle$$

- Since the "propagator" $e^{-\frac{\beta H}{L}}$ is a nonnegative matrix, every path $(x_1, ..., x_L)$ contributes a positive weight to this sum.

- Define a probability distribution on the space of paths,

$$\pi(x_1, ..., x_L) = \frac{1}{Z} \prod_{i=1}^{L} \langle x_i| e^{-\frac{\beta H}{L}} |x_{i+1}\rangle$$

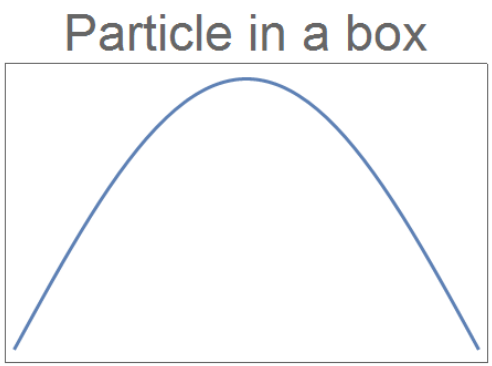
- For large β, this π has the ground state distribution as a marginal, $\psi(x)^2 = \sum_{x_2,\ldots,x_L} \pi(x, x_2, ..., x_L)$.

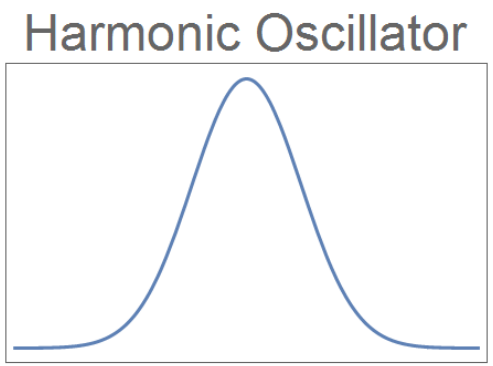
Example: spinless particles

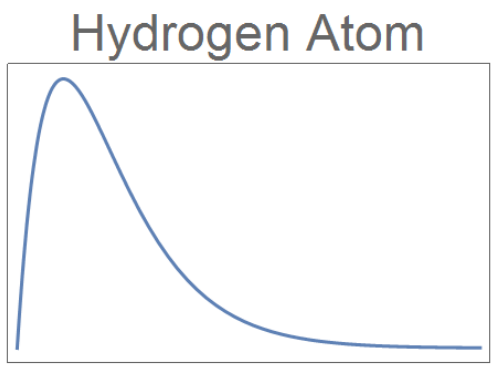
- H for a spinless particle in 1D is stoquastic in position basis,

$$H = -\partial_x^2 + V(x) \quad , \quad -\partial_x^2 \approx \begin{bmatrix} \ddots & & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & & \ddots & \end{bmatrix}$$

- Every H we teach in first year QM is stoquastic!







- Any system of interacting bosons or distinguishable particles with $H = K + U$ is stoquastic.

Example: transverse Ising model

- Transverse Ising models are stoquastic in the Z basis,

$$H = -\sum_{i=1}^{n} X_i - \sum_{i,j} Z_i Z_j \quad , \quad X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad , \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- So are generalized TIM with disordered interactions,

$$H = -\sum_{i} \Gamma_i X_i + \sum_{i,j} \alpha_{ij} Z_i Z_j + \sum_{i} b_i Z_i \quad , \quad \Gamma_i > 0$$

- Theorem: generalized TIM are universal for simulating stoquastic Hamiltonians. Proof uses perturbative gadgets. (Bravyi, Hastings '14, Cubitt, Montanaro, Piddock '16).

Hardness of solving the sign problem

- Given local H that looks nonstoquastic (has a sign problem), find a choice of basis that makes it stoquastic?

- Related to solving classical spin glasses, so it's NP-hard even in cases when it's possible. (Troyer and Wiese, '04)

- Tricks can tame sign problem in special cases. Physical systems with an 'intrinsic' sign problem?

- Double semion model (Hastings '15), Fractional quantum Hall & chiral phase of Kagome antiferromagnet (Ringel et al. '17).

Discussion for part 1

- If it weren't for fermions, would nature be stoquastic?
- Our intuition for quantum ground state geometry revolves around stoquastic H. Time to reshape the basic curriculum?
- All flux-type superconducting qubits are stoquastic. Building nonstoquastic H an underappreciated experimental challenge?
- Given a local H, how to check for 'signs' that it's stoquastic?

Part 2: Complexity results and classical simulation

Quantum adiabatic optimization (Farhi et al. '00)

- Minimize a cost function $f : \{0,1\}^n \to \mathbb{R}$ by sampling the ground state of an n-qubit Hamiltonian,

$$H_p = \sum_{z \in \{0,1\}^n} f(z)|z\rangle\langle z|$$

- Prepare the ground state of H_p by initializing the qubits in the ground state of a uniform transverse field $H_B = -\sum_{i=1}^n X_i$ and interpolating from H_B to H_p,

$$H(s) = (1-s)H_B + s\,H_p \quad , \quad 0 \le s \le 1$$

- **Adiabatic theorem:** running for time $\mathrm{poly}(n, \Delta^{-1})$, where $\Delta = \min_s E_1(s) - E_0(s)$ is the minimum spectral gap of $H(s)$, suffices to prepare the ground state of H_p.

Classically simulate stoquastic adiabatic computation?

- Classical spin glass problems are NP-complete, so the simulation should depend on the gap along the adiabatic path.
- Frustration-free stoquastic adiabatic computation can be classically simulated in $\mathrm{poly}(n)$ (Bravyi & Terhal '08).
- This is a great result, but transverse-field optimization is essentially always frustrated.
- Stoquastic AQC cannot be universal for quantum computation unless the polynomial hierarchy collapses (Bravyi et al. '06).
- It's still an open question whether stoquastic AQC can be efficiently classically simulated in general.

The stoquastic local Hamiltonian problem

- Deciding whether ground state energy is above or below some threshold is QMA-complete for general H (Kitaev '99).

- If H is stoquastic, then Merlin can send a classical witness that is verified by a classical Arthur. (Bravyi et al. '06)

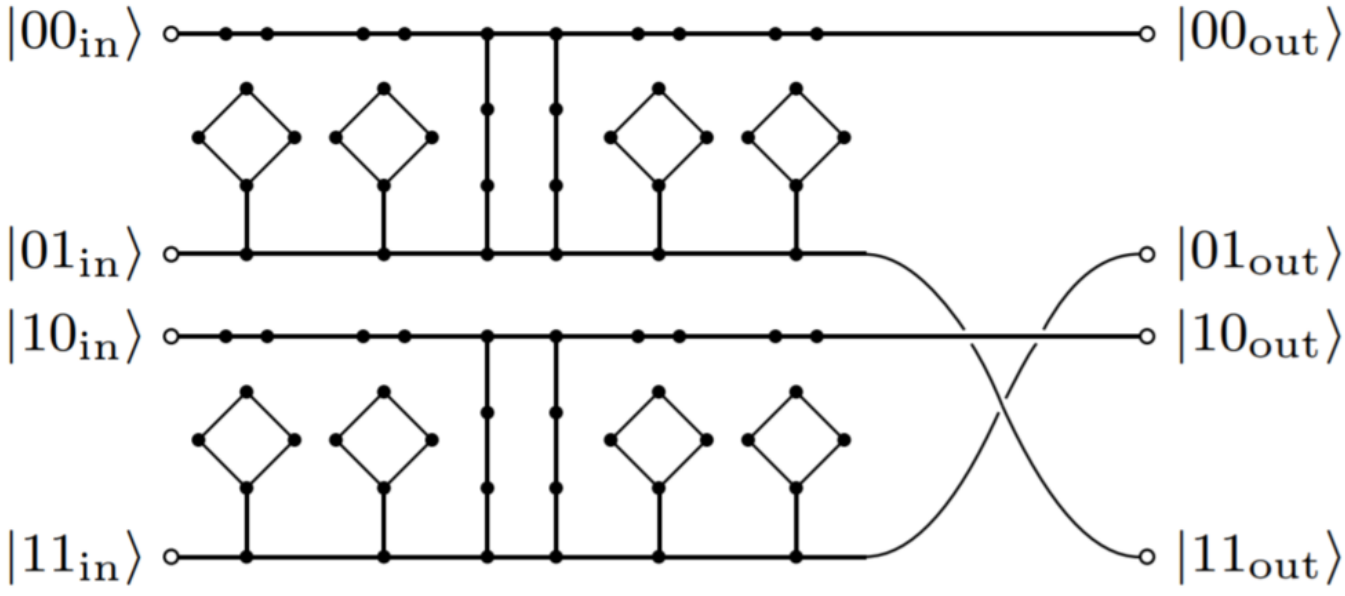
- Proof: Arthur estimates the partition function using the path integral. He estimates Z by counting a subset of bit strings, and Merlin helps him count with a hashing protocol.

- We believe AM is a strict subset of QMA, so this is evidence that stoquastic ground state problems are easier.

Universality of time evolution with stoquastic H

- Universal gate sets can be generated by stoquastic H, e.g. Hadamard + CPHASE + $\pi/8$ gate.

- Time evolution with time-independent stoquastic H is universal, by continuous-time quantum walks (Childs '08).



Universality of excited states

- Deciding excited state energies of stoquastic H is QMA-complete (Jordan, Gosset, Love '08).

- Proof: make any real H stoquastic by enlarging Hilbert space,

$$1 \to \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad , \quad -1 \to \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

- Can also be used to do universal adiabatic computation in excited states stoquastic Hamiltonians.

Classical simulation methods

- Recall that we defined a distribution on the space of paths,

$$\pi(x_1, ..., x_L) = \frac{1}{Z} \prod_{i=1}^{L} \langle x_i | e^{-\frac{\beta H}{L}} | x_{i+1} \rangle$$

- Path integral Monte Carlo (Suzuki '77): use Markov chain with Metropolis transition probabilities to sample π, and use samples to estimate quantum observables by Monte Carlo.

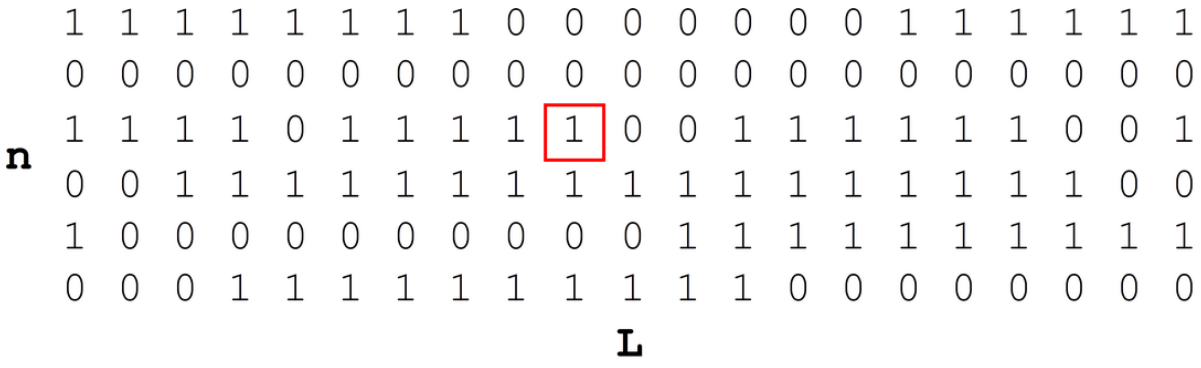
- Suzuki-Trotter approximation $e^{\epsilon(A+B)} \approx e^{\epsilon A} e^{\epsilon B}$ introduces systematic error. Take "continuous imaginary-time" $L \to \infty$.

- Another solution is to use stochastic series expansion (Sandvik '03). Instead of path integral, use Taylor series,

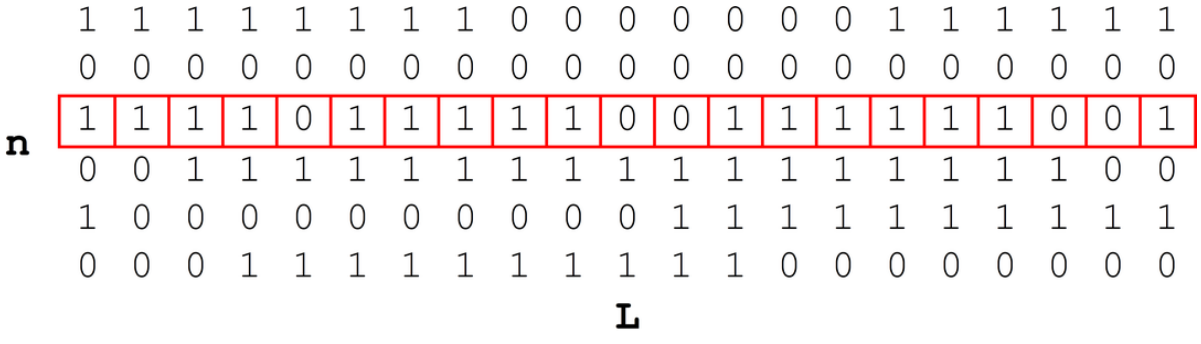
$$e^{-\beta H} = \sum_{k=0}^{\infty} \frac{(-\beta H)^k}{k!}$$

Path integral Monte Carlo

- Early simulations used single-site updates:



- "Wordline updates" speed up equilibration:



- "Worm updates", "reptation updates", "isoenergetic cluster moves", and many more reduce polynomial overhead.

Rigorous poly time simulation with PIMC

- Ferromagnetic transverse Ising models on any graph with $\beta = \mathrm{poly}(n)$ (Bravyi '14).
- Ferromagnetic XY models with local fields on any graph with $\beta = \mathrm{poly}(n)$ (Bravyi and Gosset '16).
- 1D generalized transverse Ising models up to $\beta = \mathcal{O}(\log n)$ using single-site updates (EC & Harrow, '15).
- Mean field problems with a high energy barrier using single-site updates (EC & Harrow '16, Jiang et al. '16).

Diffusion Monte Carlo

- Instead of QMC methods involving many replica slices, consider imaginary-time Schrodinger equation:

$$\frac{d}{dt}|\psi\rangle = -H|\psi\rangle \quad , \quad P_{x\to y} = \langle y|e^{-\epsilon H}|x\rangle$$

- In general $-H$ is a substochastic generator, so this evolution does not conserve probability.

- To counter this one can use a population of walkers that can reproduce or perish, or a trial wave function $\psi_T(x)$.

- Conceptually interesting, and still important in chemistry (GFMC), but not state of the art in spin systems.

Frustration-free diffusion Monte Carlo

- Classical simulation for frustration-free stoquastic $H = \sum_i \Pi_i$ inspired by diffusion Monte Carlo (Bravyi and Terhal '08).
- Define $G = I - H/\|H\|$, and define the Markov chain

$$P_{x\to y} = \frac{\langle y|\psi\rangle}{\langle x|\psi\rangle}\langle x|G|y\rangle$$

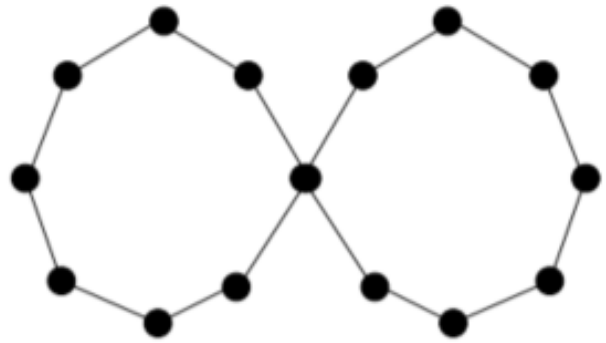
- Notice that $P_{xy} \geq 0$ and $\sum_{y\in\mathcal{B}} P_{x\to y} = 1$.
- Samples $\pi(x) = \psi(x)^2$, spectral gap $\Delta_P = \Delta_H/\|H\|$.
- Trick for computing $\langle y|\psi\rangle/\langle x|\psi\rangle$ using local projectors:

$$\frac{\langle y|\psi\rangle}{\langle x|\psi\rangle} = \sqrt{\frac{\langle y|\Pi_a|y\rangle}{\langle x|\Pi_a|x\rangle}}$$

- Classically simulates FF stoquastic AQC in time $\mathrm{poly}(n, \Delta_H^{-1})$.

Obstructions to classical simulation

- Topological obstructions: spaces with nontrivial π_1 obstruct worldline strings from equilibrating (Hastings et al. '13).



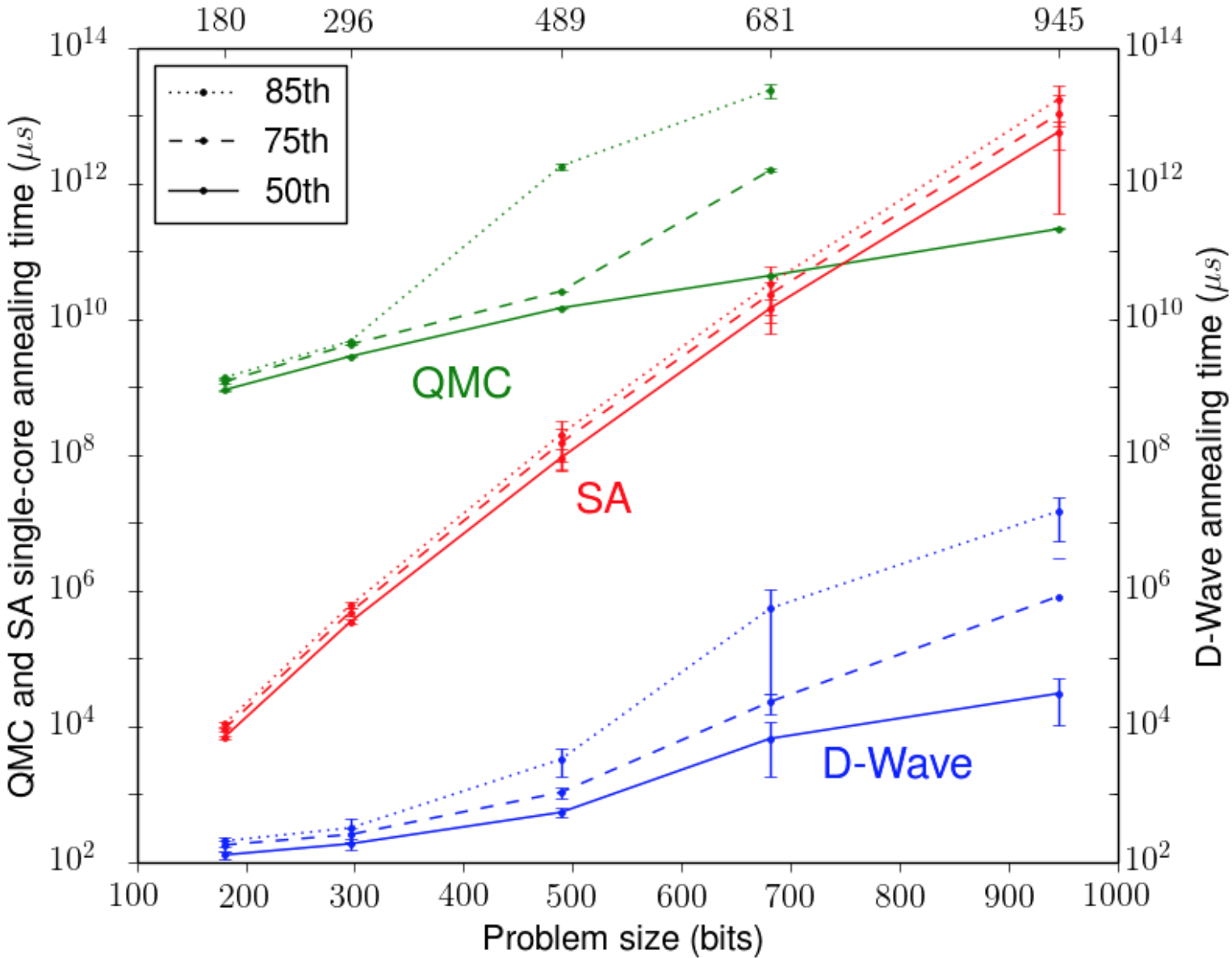
- L1 vs L2 obstructions: amplitude distribution $\psi(x)/\|\psi\|_1$ and probability distribution $\psi(x)^2$ can be far apart.

- Foils open-boundary condition PIMC (Hastings and Freedman '13) and diffusion QMC (Bringewatt et al. '17).

- At the present time there is no general purpose QMC scheme which simultaneously avoids all known obstructions.

Simulated quantum annealing

- Despite these obstructions, SQA works very well in practice:



Discussion for part 2

- Are we ever going to classically simulate stoquastic adiabatic computation in time $\mathrm{poly}(n, \Delta_H^{-1})$?

- Even if finely tuned obstructions are inevitable, can we better explain the effectiveness of PIMC in practice?

- Can we devise new QMC methods, or even ways to simulate stoquastic H beyond Markov chain Monte Carlo?