On complexity of the quantum Ising model

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Abstract

We study the computational complexity of estimating the ground state energy and simulating the adiabatic evolution for the transverse field Ising model (TIM). It is shown that the ground state energy problem for TIM on a degree-3 graph is complete for the complexity class StoqMA. This is an extension of the classical class MA where the verifier can accept quantum states as a proof and apply classical reversible gates in a coherent fashion. As a corollary, we complete the complexity classification of 2-local Hamiltonians with a fixed set of interactions proposed recently by Cubitt and Montanaro. In the special case of the ferromagnetic TIM we show that the ground state energy problem is contained in BPP. Finally, we prove that the adiabatic quantum computing (AQC) with TIM has the same computational power as AQC with general 2-local stoquastic Hamiltonians.

Calculating the ground state energy and thermal equilibrium properties of interacting quantum many-body systems is one of the central problems in quantum chemistry and condensed matter physics. It was realized early on that the complexity of this problem depends on the statistics of the constituent particles. For systems composed of bosons and for certain special classes of spin Hamiltonians the quantum partition function can be mapped to the one of a classical system occupying one extra spatial dimension [1] which often enables efficient Monte Carlo simulation [2, 3, 4, 5, 6, 7]. On the other hand, for systems composed of fermions and for the vast majority of spin Hamiltonians the quantum-to-classical mapping produces a partition function with unphysical Boltzmann weights taking both positive and negative (or complex) values — a phenomenon known as the "sign problem".

Here we focus on quantum spin Hamiltonians avoiding the sign problem also known as *stoquastic*. The defining property of stoquastic Hamiltonians is that their off-diagonal matrix elements in the standard product basis must be real and non-positive. The stoquastic class encompasses many interesting models such as TIM, the Heisenberg ferromagnetic and antiferromagnetic models (the latter is stoquastic on any bipartite graph), quantum simulated annealing Hamiltonians [8], the toric code Hamiltonian [9], and Hamiltonians derived from reversible Markov chains [10, 11, 12]. Identifying "easy" and "hard" instances of stoquastic Hamiltonians is therefore important as it could give insights on the power and limitations of classical Monte Carlo simulation algorithms [13] and contribute to our understanding of speedups in quantum annealing algorithms [14, 15].

To state our results let us define several classes of stoquastic Hamiltonians. Let $\mathsf{TIM}(n,J)$ be the set of all n-qubit transverse field Ising Hamiltonians

$$H=\sum_{u=1}^{n} h_u X_u + g_u Z_u + \sum_{1\le u<v\le n} \omega_{u,v} Z_u Z_v,$$

such that the coefficients $h_u, g_u, \omega_{u,v}$ have magnitude at most J for all u,v. Here X_u and Z_u are the Pauli operators σ^x and σ^z acting on a qubit u. Note that H is a stoquastic Hamiltonian iff $h_u \le 0$ for all u. This condition can always be satisfied by a local change of basis. A TIM Hamiltonian is said to be ferromagnetic iff $\omega_{u,v} \le 0$ for all u,v. Let $\mathsf{FTIM}(n,J) \subset \mathsf{TIM}(n,J)$ be the subclass of the ferromagnetic TIM Hamiltonians. A TIM Hamiltonian is said to have interactions of degree d iff each qubit is coupled to at most d other qubits with ZZ interactions. Our first theorem asserts that the partition function of the ferromagnetic TIM admits a fully polynomial time randomized approximation scheme (FPRAS).

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Theorem 1. *Let $\mathcal{Z} = \operatorname{Tr} e^{-H}$ be the quantum partition function corresponding to H. There exists a classical randomized algorithm that takes as input a Hamitlonian $H \in \mathsf{FTIM}(n, J)$, a precision $\delta > 0$ and outputs a random variable $\tilde{\mathcal{Z}}$ such that*

$$\Pr\Big[\,(1-\delta)\mathcal{Z} \le \tilde{\mathcal{Z}} \le (1+\delta)\mathcal{Z}\,\Big] \ge 2/3.$$

The algorithm has running time $poly(n, J, \delta^{-1})$.

The theorem immediately implies that the free energy $F(T) = -T \log\left(\operatorname{Tr} e^{-H/T}\right)$ can be approximated with an additive error ϵ in time $poly(n, J, \epsilon^{-1}, T^{-1})$. Furthermore, since $F(0) - F(T) = \int_0^T dT' S(T') \le nT$, where $S(T')$ is the entropy of the Gibbs state, we conclude that the ground state energy $F(0)$ can be approximated with an additive error ϵ in time $poly(n, J, \epsilon^{-1})$. Unfortunately, the degree of these polynomial functions is too large to have any practical implications. A rigorous upper bound on the running time obtained in the proof of Theorem 1 is $O(n^{59} J^{21} \delta^{-9})$.

Let $\mathsf{StoqLH}(n, J)$ be the set of all 2-local stoquastic Hamiltonians H on n qubits with the maximum interaction strength J. More formally, $H \in \mathsf{StoqLH}(n, J)$ iff

$$H = \sum_{1 \le u < v \le n} H_{u,v},$$

where $H_{u,v}$ is a tensor product of some hermitian operator on the qubits u, v and the identity operator on the remaining qubits, $\|H_{u,v}\| \le J$, and $\langle x|H_{u,v}|y\rangle \le 0$ for all $x \ne y$. In particular, any operator $H_{u,v}$ must have real matrix elements in the standard product basis. It can be shown that any such operator $H_{u,v}$ is a sum of a diagonal two-qubit Hamiltonian and a convex linear combination of the following interactions:

$$-X \otimes |0\rangle\langle 0|, \quad -X \otimes |1\rangle\langle 1|, \quad -X \otimes X - Y \otimes Y, \quad -X \otimes X + Y \otimes Y.$$

Our second theorem asserts that any 2-local stoquastic Hamiltonian can appear as an effective low-energy theory emerging from the TIM on a degree-3 graph.

Theorem 2. *Consider any triple ϵ, n, J where $\epsilon > 0$ is a precision, n is the number of qubits, and J is the interaction strength. There exist $n' \le \mathsf{poly}(n)$, $J' \le \mathsf{poly}(n, J, \epsilon^{-1})$, and a smooth map*

$$f \,:\, \mathsf{StoqLH}(n, J) \to \mathsf{TIM}(n', J')$$

such that the following holds for any Hamiltonian $H \in \mathsf{StoqLH}(n, J)$:
(1) The i-th lowest eigenvalues of H and $f(H)$ differ at most by ϵ for all $1 \le i \le 2^n$.
(2) One can compute $f(H)$ in time $poly(n)$.
(3) $f(H)$ has interactions of degree $d = 3$.

The theorem has important implications for classifying complexity of the Local Hamiltonian Problem (LHP) [16, 17]. Recall that LHP is a decision problem where one has to decide whether the ground state energy E_0 of a given k-local Hamiltonian H acting on n qubits is sufficiently small, $E_0 \le E_{yes}$, or sufficiently large, $E_0 \ge E_{no}$. Here $E_{yes} < E_{no}$ are some specified thresholds such that $E_{no} - E_{yes} \ge \mathsf{poly}(n^{-1})$. The Hamiltonian must have interaction strength at most $\mathsf{poly}(n)$. It is known that LHPs for 2-local and k-local stoquastic Hamiltonians have the same complexity for any constant k, modulo polynomial reductions [18]. Furthermore, LHP for 6-local stoquastic Hamiltonians is known to be a complete problem for the complexity class StoqMA [18, 19]. This is an extension of the classical class MA where the verifier can accept quantum states as a proof. To examine the proof the verifier is allowed to apply classical reversible gates in a coherent fashion and, finally, measure some qubit in the X-basis. The verifier accepts the proof if the measurement outcome is '+', see [19] for a formal definition. Combining these known results and Theorem 2 we infer that TIM-LHP is a StoqMA-complete problem. Less formally, estimating the ground state energy of TIM is shown to be as hard as estimating the ground state energy of a general k-local stoquastic Hamiltonian for

$k = O(1)$. As a corollary, we complete Cubitt-Montanaro complexity classification of 2-local Hamiltonians that can be built from a fixed set of two-qubit hermitian operators $\mathcal{S}$ [20]. The problem studied in [20] is special case of the 2-local LHP such that Hamiltonians are required to have a form $H = \sum_a x_a V_a$, where x_a is a real coefficient and V_a is an operator from $\mathcal{S}$ applied to some pair of qubits. For brevity, let us call the above problem $\mathcal{S}$-LHP. Combining the results of Ref. [20] and StoqMA-completeness of TIM-LHP one infers that depending on the choice of $\mathcal{S}$, the problem $\mathcal{S}$-LHP is is either complete for one of the complexity classes NP, StoqMA, QMA, or can be solved in polynomial time on a classical computer.

Finally, Theorem 2 offers new insights on the computational power of the adiabatic quantum computing (AQC) with TIM which received a significant attention recently [21, 22, 23]. Namely, Theorem 2 implies that AQC with TIM has the same computational power as AQC with general 2-local stoquastic Hamiltonians (modulo polynomial reductions). Indeed, suppose $\{H(s), 0 \leq s \leq 1\}$ is an adiabatic path in the space of 2-local stoquastic Hamiltonians $\mathsf{StoqLH}(n, J)$ with the minimum spectral gap δ. Choosing a precision $\epsilon = \delta/3$ and applying the mapping of Theorem 2 one gets a new adiabatic path $f(H(s)) \in \mathsf{TIM}(n', J')$ with the minimum spectral gap at least $\delta/3$. Assuming that $J \leq \mathsf{poly}(n)$ and $\delta \geq \mathsf{poly}(n^{-1})$, one infers that $J' \leq \mathsf{poly}(n)$, that is, the new adiabatic path can be traversed in time $\mathsf{poly}(n)$, see the supplemental material for more details.

Proof strategy: Theorem 1 is a simple application of the seminal result by Jerrum and Sinclair [24] who showed that the partition function of the ferromagnetic *classical* Ising model admits FPRAS. To prove Theorem 1 we employ the standard quantum-to-classical mapping based on the Suzuki-Trotter formula. The only new ingredient that we add is a proof that the Suzuki-Trotter approximation leads to a small *multiplicative* error (as opposed to the additive error usually studied in the literature). A complete proof of Theorem 1 can be found in [25].

To prove Theorem 2 we employ perturbative reductions [17, 26] and the Schrieffer-Wolff transformation [27, 28, 29]. At each step of the proof we work with two quantum models: a high-energy simulator Hamiltonian $H_{\rm sim}$ acting on some Hilbert space $\mathcal{H}$ and a low-energy target Hamiltonian $H_{\rm target}$ acting on some subspace $\mathcal{H}_- \subseteq \mathcal{H}$. We show that $H_{\rm target}$ can be obtained from $H_{\rm sim}$ as an effective low-energy Hamiltonian calculated using a few lowest orders of the perturbation theory. We apply the above step recursively several times such that the target Hamiltonian at the t-th step becomes the simulator Hamiltonian at the $(t+1)$-th step. The recursion starts from the TIM with interactions of degree-3 at the highest energy scale, goes through several intermediate models listed below, and terminates at a given 2-local stoquastic Hamiltonian at the lowest energy scale.

1	TIM, degree-3 graph
2	TIM, general graph
3	Hard-core dimers, triangle-free graph
4	Hard-core bosons, range-2
5	Hard-core bosons, range-1
6	Hard-core bosons, range-1, controlled hopping
7	2-local stoquastic Hamiltonians

The hard-core bosons (HCB) model describes a multi-particle quantum walk on a graph. The Hamiltonian consists of a hopping term, on-site chemical potential, and arbitrary two-particle interactions. Different particles must be separated from each other by a certain minimum distance that we call a range of the model. HCB is closely related to the Bose-Hubbard model. The hard-core dimers model is analogous to HCB except that admissible particle configuration must consist of nearest-neighbor pairs of particles that we call dimers. Different dimers must be separated from each other by a certain minimum distance. To reduce the degree of interactions in TIM we encode each qubit of the target model into the (approximately) two-fold degenerate ground subspace of the one-dimensional TIM on a chain of a suitable length. A rigorous definition of the above models and a complete proof of Theorem 2 are provided in the supplemental material.

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