Approximation Guarantees for the Quantum Local Hamiltonian Problem and Limitations for Quantum PCPs

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Motivation and Background: A quantum k-local Hamiltonian on n qudits is a $d^n \times d^n$ Hermitian matrix H of the form

$$H = \sum_{i=1}^{m} H_i, \tag{1}$$

where each term H_i acts non-trivially on at most k qudits and $\|H_i\| \leq 1$. Local Hamiltonians are ubiquitous in physics, where interactions are almost always few-body. Of particular interest, e.g. in condensed matter physics, is to understand the low-energy properties of local Hamiltonians. A benchmark problem, termed the local Hamiltonian problem, is to approximate the ground-state energy (i.e. the minimum eigenvalue) of the model. What is the computational complexity of this task?

In a seminal result Kitaev proved that the local Hamiltonian problem is complete for the quantum complexity class QMA, in the regime of estimating the energy to within polynomial accuracy in the number of particles of the model [2]. Kitaev's result has been developed into a new area around the question of understanding the computational complexity of local Hamiltonians, at the crossover of quantum complexity theory and condensed matter physics: quantum Hamiltonian complexity [9].

The local Hamiltonian problem can be seen as a quantum analogue of constraint satisfaction problems (CSPs) and Kitaev's result as a quantum version of the Cook-Levin theorem. Let unsat($\mathcal{C}$) be the fraction of the total number of local constraints that are not satisfied in the best possible assignment for $\mathcal{C}$. Then one formulation of the Cook-Levin theorem is that it is NP-hard to compute unsat($\mathcal{C}$) for an arbitrary CSP $\mathcal{C}$. However this leaves open the possibility that one might be able to approximate unsat($\mathcal{C}$) to within small error in reasonable time.

The objective of the theory of approximation algorithms is find out in which cases one can obtain in polynomial time approximate solutions to problems that are hard to solve exactly. This is by now a well developed theory [10]. The quantum case, in contrast, is largely unexplored (see however [11–14]). It is also interesting to understand what are the limitations for obtaining approximation algorithms; this is the goal of the theory of hardness of approximation, where one is interested in proving the computational hardness of obtaining even approximate solutions. A landmark result in this theory, on which almost all other hardness of approximation results are based, is the PCP Theorem [15–17]. One possible formulation is in terms of 2-CSPs and states: There is a constant $\varepsilon_0 > 0$ such that it is NP-hard to determine whether for a given 2-CSP $\mathcal{C}$, unsat($\mathcal{C}$) $= 0$ or unsat($\mathcal{C}$) $\geq \varepsilon_0$.

As well as developing a quantum theory of approximation algorithms, a theory of hardness of approximation for QMA would also be an interesting development. Inspired by the PCP theorem we might be tempted to speculate a quantum hardness of approximation result for the local Hamiltonian problem. Consider a local Hamiltonian $H = \sum_{i=1}^{m} H_i$, and denote the minimum eigenvalue of H by $E_0 = E_0(H)$. The mean ground-state energy is defined by $e_0(H) := \frac{E_0(H)}{m}$. The mean ground-state energy is the quantum analogue of the unsat value of CSPs. A central open problem in quantum Hamiltonian complexity is the following [9, 13, 14, 18–21]:

Conjecture 1 (Quantum PCP Conjecture)**.** *There is a constant $\varepsilon_0 > 0$ such that it is* QMA*-hard to decide whether for a 2-local Hamiltonian H, $e_0(H) = 0$ or $e_0(H) \geq \varepsilon_0$.*

One could also consider the conjecture for k-local Hamiltonians. However it has been proved that Conjecture 1 is equivalent to this more general version, even when restricted to 2-local Hamiltonians with sites formed by qubits [20].

A way to refute the quantum PCP conjecture is to show that the estimation of the mean ground-state energy can be realized in NP. In [1] we follow this approach and give new approximation guarantees for the local Hamiltonian problem in the regime of extensive error.

Statement of Main result: The main result of our paper [1] shows that one can obtain a good approximation to the mean ground-state energy by a product state (after coarse-graining some of the sites) for a large class of 2-local Hamiltonians. To every 2-local Hamiltonian we can associate a constraint graph $G = (V, E)$ with V the set of vertices associated to the sites of the Hamiltonian, and E the set of edges associated to the interaction terms of the Hamiltonian. Given a graph $G = (V, E)$ and a subset of vertices S, we define the expansion of S as $\Phi_G(S) := \Pr_{(u,v)\in E}(v \notin S | u \in S)$. The expansion of the graph G is defined as $\Phi_G := \min_{S:|S|\leq|V|/2} \Phi_G(S)$.

Theorem. *Let H be a 2-local Hamiltonian on n d-dimensional particles defined on a regular graph $G = (V, E)$ of degree deg(G). Then for every state ρ, integer $m \geq 1$, and every partition of the vertices into sets $\{X_i\}_{k=1}^{n/m}$, each composed of m particles, there is a product state $|\psi_1, \ldots, \psi_{n/m}\rangle$ (with $|\psi_i\rangle$ a state on the space associated to X_i) such that*

$$\frac{1}{|E|}\langle\psi_1, \ldots, \psi_{n/m}|H|\psi_1, \ldots, \psi_{n/m}\rangle \leq \frac{1}{|E|}\operatorname{tr}(H\rho) + 8\left(\frac{36\ln(2)d^6\mathbb{E}_i\Phi_G(X_i)}{deg(G)}\frac{\mathbb{E}_i I(X_i : X_i^c)_\rho}{m}\right)^{1/6}, \quad (2)$$

where $I(X_i : X_i^c)_\rho$ the mutual information of X_i with its complementary region X_i^c in the state ρ.

In particular choosing $\rho = \psi_0$, with $\psi_0 := |\psi_0\rangle\langle\psi_0|$ the projector onto a groundstate $|\psi_0\rangle$ of H,

$$\frac{1}{|E|}\langle\psi_1, \ldots, \psi_{n/m}|H|\psi_1, \ldots, \psi_{n/m}\rangle \leq e_0(H) + 8\left(\frac{36\ln(2)d^6\mathbb{E}_i\Phi_G(X_i)}{deg(G)}\frac{2\mathbb{E}_i S(X_i)_{\psi_0}}{m}\right)^{1/6}, \quad (3)$$

where $S(X_i)_{\psi_0}$ is the von-Neumann entropy of $\operatorname{tr}_{X_i^c}(\psi_0)$, with $\operatorname{tr}_{X_i^c}$ the partial trace over all sites in X_i^c.

The theorem gives a non-trivial approximation in terms of three parameters: the average expansion of the regions X_i, the degree of the graph, and the average entanglement of the regions X_i with their complement. Below we discuss the relevance of last two of them (since the first is a well-known fact).

Degree of the Graph: An easy consequence of the PCP theorem [15–17] is the following fact: For any constants $c, \alpha, \beta > 0$, it is NP-hard to determine whether a 2-CSP $\mathcal{C}$, with alphabet Σ on a constrained graph of degree deg, is such that unsat$(\mathcal{C}) = 0$ or unsat$(\mathcal{C}) \geq c|\Sigma|^\alpha/\text{deg}^\beta$.

Assuming QMA $\not\subseteq$ NP, the theorem shows the analogous result for the quantum case – namely that it is QMA-hard to achieve a $cd^\alpha/\text{deg}^\beta$ approximation for the mean ground-state energy of 2-local Hamiltonians – is *not* true. This suggest a route for a disproof of the quantum PCP conjecture by trying to a find a procedure for increasing the degree of the constraint graph without decreasing the mean ground-state energy of the model (by possibly increasing the dimension of the particles as well). Classically this can be achieved by parallel repetition of the CSP (see Prop. 4 of [1]), but it is unclear whether there is an analogous construction in the quantum case.

The approximation in terms of the degree can be interpreted as an instance of monogamy of entanglement [22], a feature of quantum correlations that says a system cannot be highly entangled with a large number of other systems. If the degree is high, it means that every particle is connected to many others by an interaction term. But since it cannot be highly entangled with many of them, we might expect that a product state gives a reasonable approximation to the energy of most such interactions. Indeed based on this idea it is folklore in condensed-matter physics that

mean field (where one uses a product state as an ansatz to the groundstate) becomes exact once the dimension of the interaction lattice increases. The approximation we obtain here in terms of the degree of the graph gives a rigorous justification to this intuition. Finally the result also gives an approximation for *highly expanding* graphs by using the bound $\Phi_G \leq 1/2 - \Omega(\deg^{-1/2})$ relating the expansion and the degree. Thus graphs with almost maximum expansion $\Phi \to 1/2$ are not candidates for QMA-hard instances.

Average Entanglement: The theorem shows that we can obtain a classical proof of size $O(n2^{O(m)})$ that proves $e_0(H)$ to be small whenever the groundstate satisfies a subvolume law for entanglement, i.e. whenever we can find a partition of the sites into regions X_i of size m such that in the groundstate their entanglement (with the complementary region) is sublinear in the number of particles of the region.

There is a general intuition that the amount of entanglement in the groundstate of a Hamiltonian should be connected to its computational complexity (see e.g. [24]), which can be made precise in 1D assuming an area law for entanglement. Here we find a similar situation, but with important differences. On one hand the result is weaker in that it only implies an efficient classical description of the groundstate for estimating the mean ground-state energy; on the other hand the result is much more general, being true for 2-local Hamiltonians on general interaction graphs and only requiring a subvolume law instead of an area law. This new relation of entanglement and computational hardness gives a motivation for studying the entanglement scaling in groundstates of Hamiltonians on more general graphs than finite dimensional ones.

Another interesting choice for the state ρ in Theorem is the thermal state of the Hamiltonian at temperature T: $\rho_T := \exp(-H/T)/\operatorname{tr}(\exp(-H/T))$. Using the bound $|E|^{-1}\operatorname{tr}(H\rho_T) \leq e_0(H) + \varepsilon$ for $T = O(d^{-1}\varepsilon)$ we find there are states satisfying $\frac{1}{|E|}\langle\psi_1, ..., \psi_{n/m}|H|\psi_1, ..., \psi_{n/m}\rangle \leq e_0(H) + \varepsilon + 8\left(\frac{36\ln(2)d^6\mathbb{E}_i\Phi_G(X_i)}{\deg(G)}\frac{\mathbb{E}_i I(X_i:X_i^c)_{\rho_T}}{m}\right)^{1/6}$. Therefore Hamiltonians for which the thermal state satisfies a subvolume law for the mutual information for constant, but arbitrary small, temperatures are also not candidates for QMA-hard instances. We find this observation interesting since it is much easier to prove area laws for thermal states than for groundstates [25].

The approximation in terms of the average mutual information means that in order for the quantum PCP conjecture to be true we must find a family of Hamiltonians on qubits whose groundstate satisfy a strict volume law for the mutual information of every region of size $n^{o(1)}$. To the best of our knowledge there is no known example of a Hamiltonian with this property. Thus to find one emerges as a natural problem if one is willing to prove the quantum PCP conjecture. In turn, proving that no such family of Hamiltonians exists would entail a disproof of the conjecture.

Other Results: In the paper [1] we also give polynomial-time algorithms for approximating the mean ground-state energy of two classes of models: (i) 2-local Hamiltonians on planar graphs of arbitrary degree, and (ii) dense k-local Hamiltonians for any k. These existence of these two algorithms solve open problems from [11] and [12], respectively.

Techniques: The proofs of our results are based on information theory. We explore the idea that given a multipartite quantum state, by measuring a few of the subsystems one can make all sufficiently small subset of subsystems close to *product*, on average over the choice of subsystems. This result, which can be seen as a version of the de Finetti theorem for arbitrary, non-symmetric, states is proved by information-theoretic methods, in particular the chain rule of mutual information.

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