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The Complexity of Estimating Local Physical Quantities

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Introduction

Computational complexity theory has proven useful in the study of physically motivated problems. We study several such natural problems in the context of the class $P^{QMA[log]}$, a class introduced by Ambainis [1].

Prior Work:

APX-SIM (Ambainis [1]): Given a *k*-local Hamiltonian *H* and an *l*-local observable *A*, estimate $\langle A \rangle := \langle\psi|A|\psi\rangle$, for $|\psi\rangle$ the ground state of *H*.

$P^{QMA[log]}$ ([1]):
The class of problems decidable in polynomial time, given a *logarithmic* number of queries to a QMA oracle.

Theorem ([1]): APX-SIM is $P^{QMA[log]}$-complete for *log*-local Hamiltonians *H* and log-local observables *A*.

We ask:

- Can the locality of the results from [1] be improved?
- What other natural problems are characterized by $P^{QMA[log]}$?
- What bounds exist on the class $P^{QMA[log]}$?

Motivation:
The study of $P^{QMA[log]}$ and related physically motivated problems offers insight into the tractability of fundamental tasks involving Hamiltonians, beyond the paradigm of estimating ground state energies.

Main Results

Theorem 1: APX-SIM and APX-2-CORR are $P^{QMA[log]}$-complete even for *1*-local observables and *5*-local Hamiltonians (on qubits).

- APX-2-COR: Estimating two-point correlation functions against a ground state. Introduced in this work.
- *Moral:* Resolves an open question of Ambainis [1] by showing that measuring just a *single* qubit of the ground space is intractable!

Theorem 2: $P^{QMA[log]} \subseteq PP$.

- PP: Decision problems solvable in probabilistic polynomial time given unbounded error.
- *Moral: Shows* $P^{QMA[log]}$ is only "slightly harder" than QMA, and improves the known containment QMA ⊆ PP [2] (i.e. we show QMA ⊆ $P^{QMA[log]} \subseteq PP$).

Theorem 3: SPECTRAL-GAP is $P^{UQMA[log]}$-hard.

- UQMA: QMA with promise of a unique accepting proof in YES case.
- *Remarks:* Ref. [1] claimed this result under many-one reductions.
- *Moral:* We identify a flaw in [1]'s proof, which assumed all queries to the QMA oracle are "valid", i.e. satisfy the "promise" of the promise problem. Building on [1], we introduce a "query validation" technique to obtain hardness under poly-time Turing reductions.

APX-SIM Hardness

The methods for showing $P^{QMA[log]}$-hardness for APX-SIM and APX-2-CORR are similar.

Proof sketch of Theorem 1 for APX-SIM:
Key idea: Think of oracle query responses as a "proof," and enforce correct computation.

1. Given a $P^{QMA[log]}$ circuit *U*, suppose it does not make oracle queries, but reads (claimed) oracle query results from a *log*-size *proof* register *Q*.
2. Plug *U* into the Kitaev-Feynman circuit-to-Hamiltonian construction [3] to obtain a *5*-local Hamiltonian H_1.
3. To force Q to encode correct query responses, construct a modified version of Ambainis's "query Hamiltonian" H_2 [1] to act on Q.
4. Set the final Hamiltonian to $H = H_1 + H_2$, and the *1*-local observable to measure the output qubit of H_1 in the standard basis.

Intuition: If "proof register" *Q* is set correctly, then the ground state of H_1 is the history state encoding *U*'s action. Forcing *Q* to be set correctly is achieved by H_2. Thus, the output qubit of H_1 encodes the answer of computation *U*, measurable by a *1*-local observable.

Contrast: The original construction of [1] simulates *U* on all $2^{O(\log n)}$ possible strings of query answers, retaining those which lead to a YES output using *A*. Then, using a clever construction in H_2, [1] checks if any such string contains correct query answers. This encoding was *log*-local.

$P^{QMA[log]} \subseteq PP$

Proof sketch of Theorem 2:
Key idea: Exploit technique of hierarchical voting, previously used to show $P^{NP[log]} \subseteq PP$ [4]. We must generalize the approach to the case of non-perfect completeness and soundness, as well as *invalid* queries.

Remarks: Protocol is natural generalization of [4] combined with strong QMA error reduction [5]. Our main contribution is its analysis, which is considerably more involved as QMA deals with *promise* problems.

We give a PQP protocol (PQP = PP [6]):

1. Attempt to "guess" the correct string of query answers $y = y_1 \dots y_m$.
2. For i from 1 to $2^m - 1$:
   - If $|y| < i$, then with probability $1 - 2^{-O(n)}$, terminate and output a bit in $\{0,1\}$ at random. Else, continue.
3. Run the $P^{QMA[log]}$ circuit on *y* and output the answer.

Intuition:

- Classically [4], the lexographically largest string *y* attainable by PP protocol is *the* correct query string. Hierarchical voting ensures *y* has the highest probability of being output.
- Quantumly, this first intuition *fails* due to possibility of invalid queries violating the QMA promise gap! In particular, for any invalid query, we have no *strong bounds* on the acceptance probability of verifier.
- *Solution*: Carefully partition and analyze strings *y* attainable in PQP protocol. First, prove weighting provided by hierarchical voting suffices despite the non-perfect error and correctness. Then, show a correct string *y* succeeds despite even *invalid* queries.

SPECTRAL-GAP Hardness

SPECTRAL-GAP: Given a local Hamiltonian, estimate its spectral gap.

Theme: Query calls to a QMA oracle must account for the possibility of *invalid* queries (i.e. violating promise of oracle). Following [7], we require the $P^{QMA[log]}$ machine to output the *same* result, no matter the response to any *invalid* queries. This issue was missed in [1].

Problem: Ref. [1] claimed $P^{UQMA[log]}$-hardness for SPECTRAL-GAP; this proof fails if invalid queries are allowed (in particular, invalid queries can close the spectral gap of the Hamiltonian constructed).

Proof sketch of Theorem 3:
Key idea: While a P machine alone cannot detect invalid queries, multiple calls to a SPECTRAL-GAP oracle can be used for this purpose.

1. Begin with [1]'s Hamiltonian construction *H*, which encodes all possible queries the $P^{UQMA[log]}$ circuit makes to the UQMA oracle.
2. *Query validation:* Carefully exploiting the precise construction of *H* allows us to use the SPECTRAL GAP oracle multiple times to estimate the spectral gap of each query Hamiltonian. If the gap is "too small," we label this query as *invalid* and discard it.

Moral: (1) Estimating spectral gaps, a fundamental problem in condensed matter physics, is intractable. *(2)* Queries to promise classes, such as QMA and UQMA, must be handled delicately.

Discussion

We studied the complexity of several problems involving local Hamiltonians beyond the standard paradigm of estimating ground state energies in Quantum Hamiltonian Complexity.

Open Questions:

- Do our results for APX-SIM and APX-2-CORR hold even for *2*-local Hamiltonians, for local Hamiltonians on a 2D lattice, or for other physically motivated Hamiltonian models?
- SPECTRAL-GAP is $P^{UQMA[log]}$-hard – is it also *complete?* Or could it be complete for $P^{QMA[log]}$? (*note:* It is contained in $P^{QMA[log]}$ [1])
- $P^{QMA[log]}$ turns out to be a natural class given the fundamental problems it characterizes. What other physically motivated tasks are captured by $P^{QMA[log]}$?

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