The importance of the spectral gap in estimating ground-state energies

Abhinav Deshpande

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Joint work with Alexey Gorshkov and Bill Fefferman

arXiv: 2007.11582

Joint Center for Quantum Information and Computer Science

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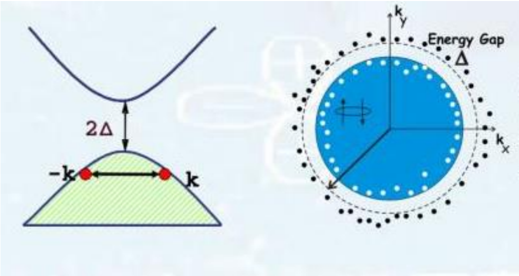
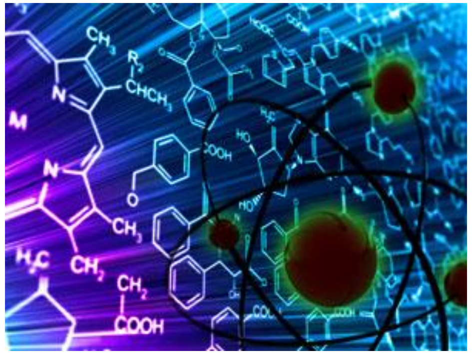
The University of Chicago 1890

Motivation

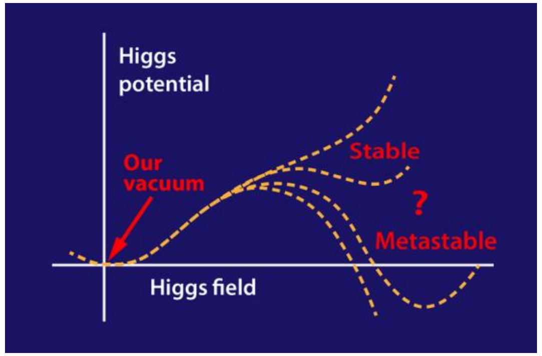
Studying ground states



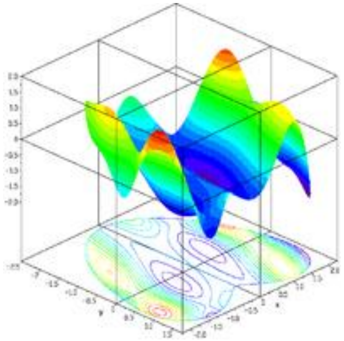
Jure Kokalj
Condensed-matter physics



Quantum chemistry



APS/Alan Stonebraker
High-energy physics



Optimisation

Exactly what many quantum algorithms aim to do!

How feasible is this for general Hamiltonians?
- Complexity theory (hardness)
- Algorithms (easiness)

Hamiltonian complexity

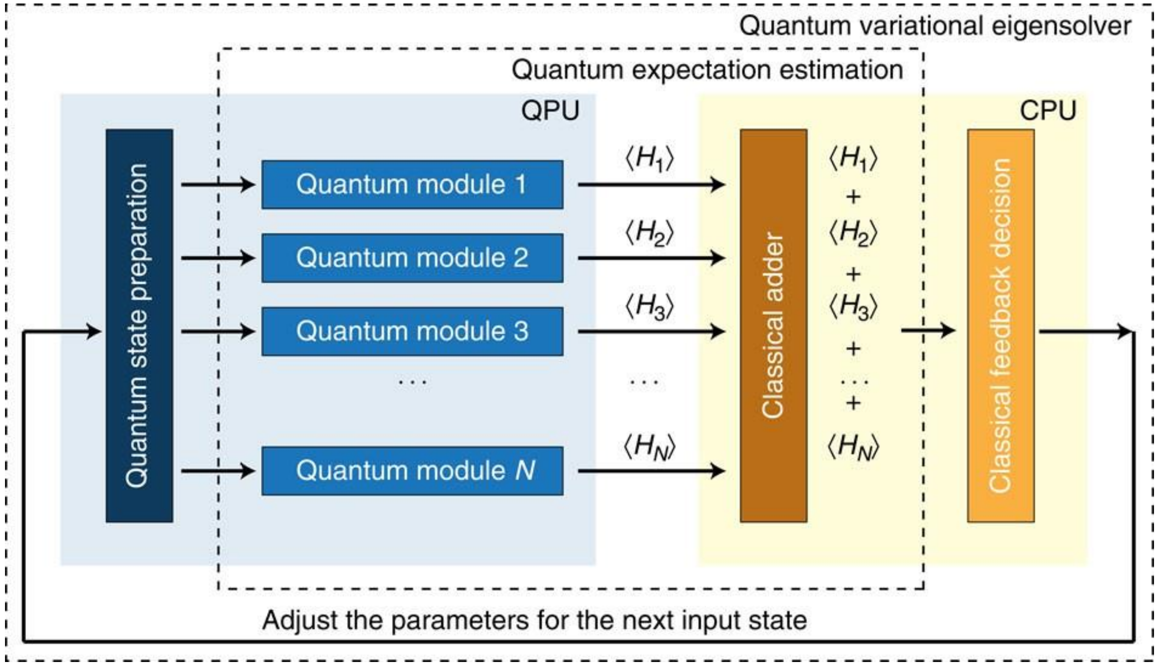
- Local Hamiltonian problem
- Input: a description of an n-qubit Hamiltonian $H = \sum_i h_i$, where each term h_i acts on at most k qubits
- Output: ground-state energy of H
- Kitaev's result[1,2]: QMA-hard to $1/\mathrm{poly}(n)$ additive error
- QMA a quantum generalisation of NP: unlikely that quantum computers can solve this problem in general
- More recent work[3]: PSPACE-hard for $1/\exp$ additive error

"Precise regime"

[1] Kitaev, Shen, Vyalyi (2002)
[2] Kempe, Kitaev, Regev, arXiv:quant-ph/0406180.
[3] Fefferman and Lin, arXiv:1601.01975, arXiv:1604.01384

Algorithms

- Efficient algorithms for special cases
  - 1D + spectral gap[1]
  - Given state with high overlap + spectral gap[2,3] [Friday 4B]
- Heuristic algorithms have been developed for other cases (most notably, VQE[4])

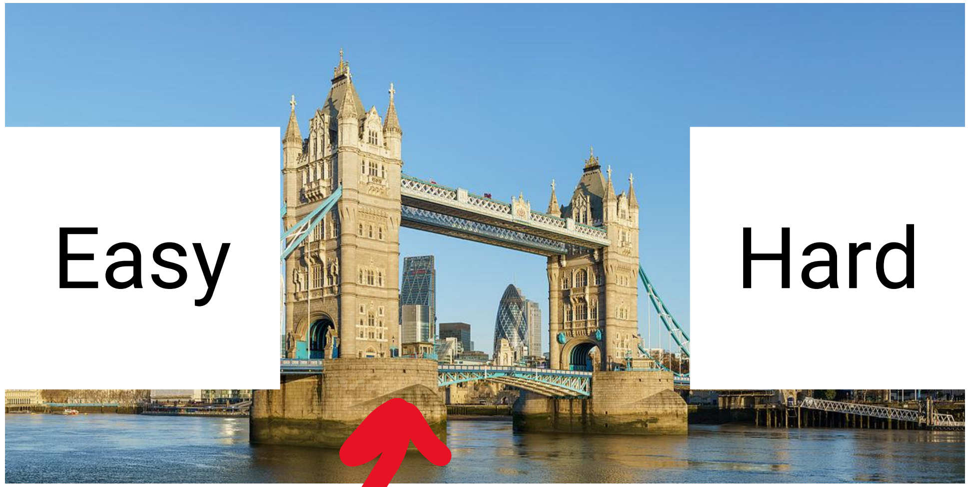


How do these results fit in with hardness?

[1] Landau, Vazirani, Vidick, Nat. Phys. (2015)
[2] Ge, Tura, and Cirac, J. Math. Phys. (2019)
[3] Lin and Tong, Quantum 4, 372 (2020)
[4] A. Peruzzo et al., Nat. Comm. 5, 4213 (2014)

Bridging easiness/hardness results

- Original hardness result is too general
- Hardness persists even for Hamiltonians with restrictions[1-4]
  - qudits in 1D[1]
  - qubits in 2D[2]
  - Translation-invariant Hamiltonians*[3]
  - Particular models[4] (Heisenberg, Bose-Hubbard[5], etc.)
- Identify structural property
  - Void generic hardness results
  - Exploitable by algorithms



[1] Aharonov et al. arXiv:0705.4077
[2] Oliveira and Terhal, arXiv:quant-ph/0504050
[3] Gottesman and Irani, arXiv:0905.2419
[4] Cubitt and Montanaro, arXiv:1311.3161
[5] Childs, Gosset, and Webb, arXiv:1311.3297

Results: two ways of adding structure

Structural property 1: spectral gap

- Many "interesting" Hamiltonians have a spectral gap
- Often associated with tensor networks and area laws[1] (proven in 1D)
- Easiness
  - Adiabatic algorithm (minimum spectral gap)
  - Efficient computation of ground-state energies[2] in 1D
- Hardness
  - More generally, do not know if hardness results can be made to survive even a $\Omega(1/\text{poly})$ spectral gap[3,4,5]
    - Clock construction not malleable
  - Our work[6]: initial piece of evidence that spectral gap makes problem easier in general

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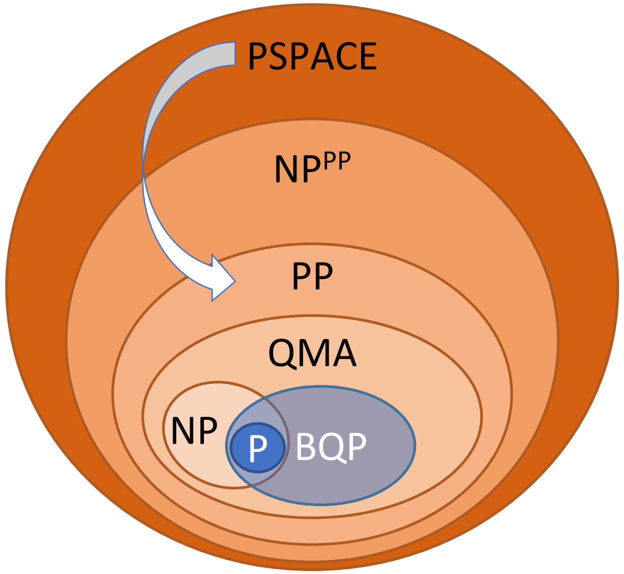
[1] M. Hastings, J. Stat. Mech., 08024 (2007)
[2] Landau, Vazirani, Vidick, Nat. Phys. (2015)
[3] González-Guillén and Cubitt, arXiv:1810.06528
[4] Crosson and Bowen, arXiv:1703.10133
[5] Aharonov et al., arXiv:0810.4840
[6] A. D., Gorshkov, and Fefferman, arXiv:2007.11582

Main result 1

- Provable setting where the spectral gap affects the complexity
- Informally: compute ground-state energy of Δ-gapped Hamiltonian to inverse-exponential precision

- $\Delta = 0$ case (no promise): PSPACE-complete[1]
- We show: $\Delta = \Omega(1/\text{poly})$ case is PP-complete.

Result 1
The spectral gap provably makes the problem easier* in this setting



*: from very, very hard (PSPACE) to very hard (PP)

- Weak evidence it's true in general

[1] Fefferman and Lin, arXiv:1601.01975, arXiv:1604.01384

Structural property 2: classical description of ground state

- In condensed-matter physics, we often want *nontrivial*, poly-size classical descriptions of ground states from which we can efficiently compute properties.
  - Tensor-network descriptions
  - Circuit to prepare ground state
- Do such descriptions always exist for local Hamiltonians?
- If yes, then QMA=QCMA
- Oracle evidence that they are different[1,2]
- How rich is the set of states with polynomial circuit complexity?

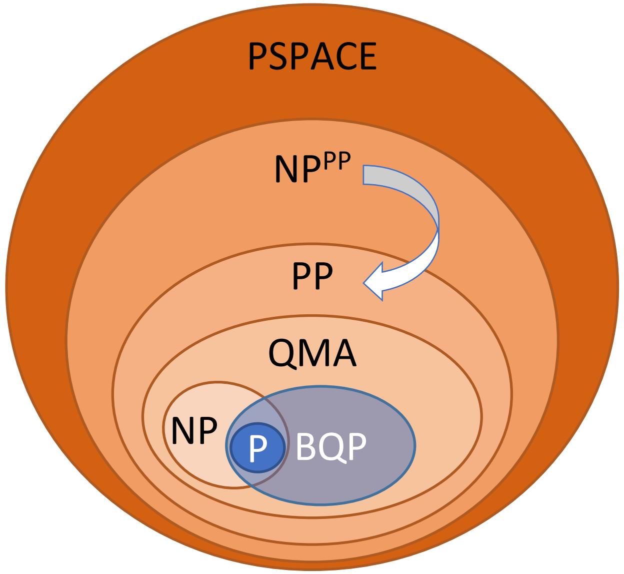
Image: ya-webdesign.com

[1] Aaronson and Kuperberg, arXiv:quant-ph/0604056 [2] Fefferman and Kimmel, arXiv:1510.06750

Main result 2

- How important is a classical description if there's also a 1/poly spectral gap?
- Not important (again in regime of inverse-exponential precision)
- In particular, $\Delta = \Omega(1/\text{poly})$ + classical-description case is again PP-complete.

Result 2
Promise of low circuit-complexity makes no difference if spectral-gap promise is already present



[1] Fefferman and Lin, arXiv:1604.01384 [2] Morimae and Nishimura, arXiv:1704.01514 [3] Gharibian et al., arXiv:1805.11139

An interesting conjecture

- A candidate explanation for Result 2

Conjecture
Spectral gap of $\Omega(1/\mathrm{poly})$ implies (nonuniform) polynomial-size circuit to prepare low-energy state

- Conjecture implies most natural Hamiltonians have short circuits to prepare their ground states!
- Would explain why variational algorithms seem to perform well
- Conjecture would imply QMA=QCMA in presence of spectral gap
  - (We have proved this for the Precise- versions of these classes)

Proof ideas

- PP upper bound
  - Prepare a thermal state at low enough temperature
  - Spectral gap ensures exponentially good overlap
  - Feynman path integral can be computed in PP
- PP lower bound
  - Modification of Aharonov et al. construction for universality of adiabatic quantum computing
  - Small-penalty clock construction
- Small-penalty clock construction: a technique that allows one to use perturbation theory, keep track of eigenvalues, and lower-bound spectral gap of the full Hamiltonian

Outlook

Spectral gap (Δ)	Classical witness	Quantum witness
$\Delta = 1/\text{poly}$	PP-complete	PP-complete
$\Delta = 0$	NP^{PP}-complete	PSPACE-complete

- Spectral gap can make the problem easier
- Conjecture: spectral gap implies polynomial-size circuit?
- Would explain why VQE works so well in practice!
- Open questions
  - Constant spectral gap
  - Non-precise regime
  - Connections to area-laws, tensor-network representations

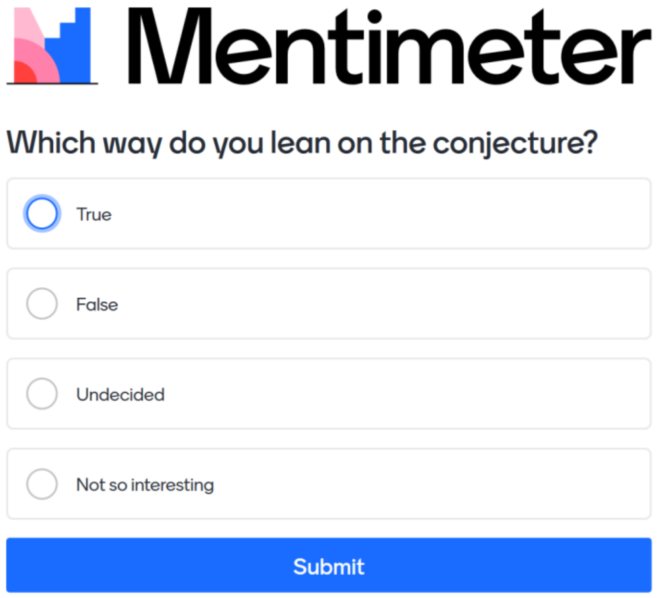
Poll

Conjecture
Spectral gap of $\Omega(1/\mathrm{poly})$ implies (nonuniform) polynomial-size circuit to prepare low-energy state

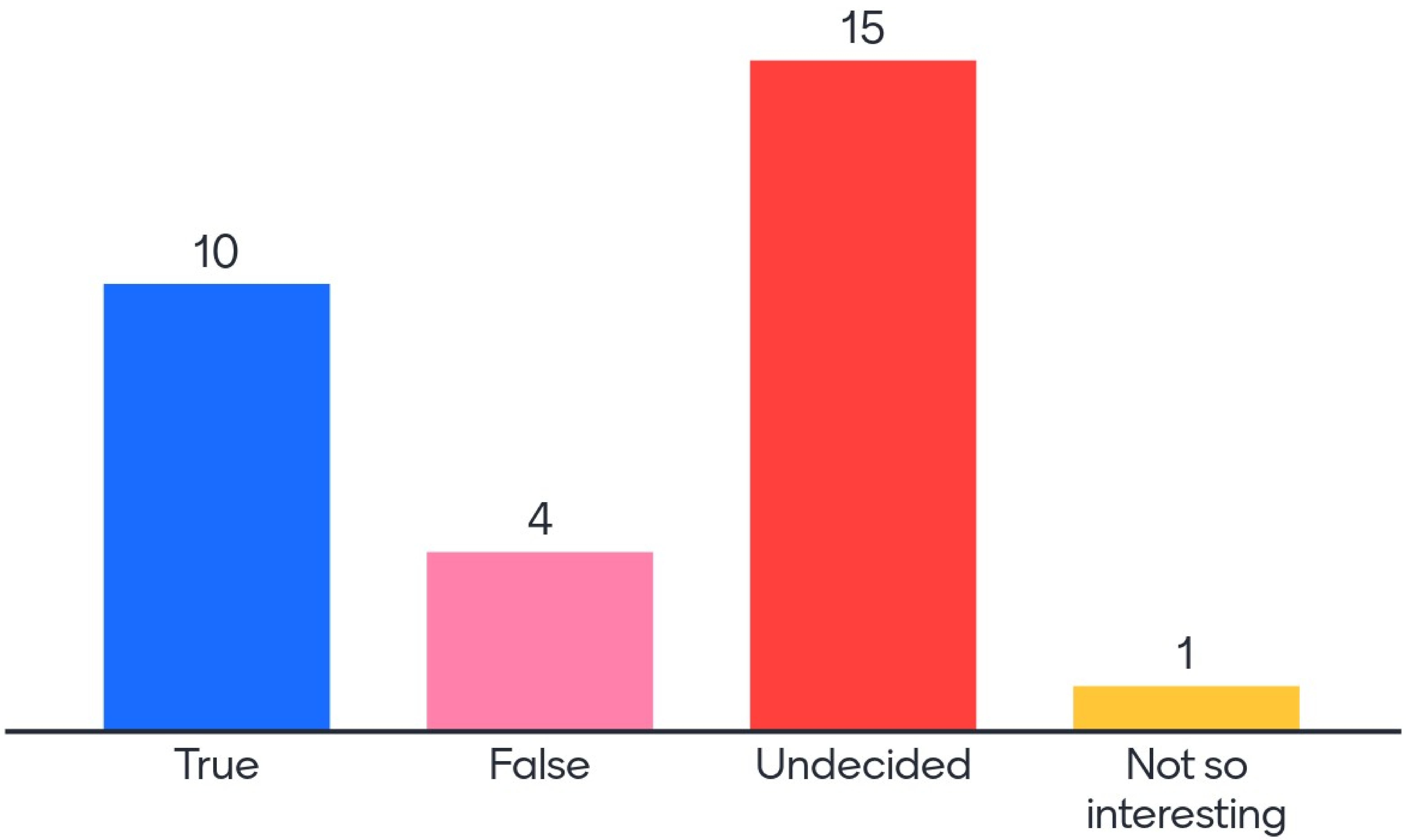
Which way do you lean on the conjecture displayed here?

(a) True
(b) False
(c) Undecided
(d) Not so interesting

Please go to ter.ps/sdx and vote there



Which way do you lean on the conjecture?



Thank you!

Appendix

PGQMA and PrecisePGQMA

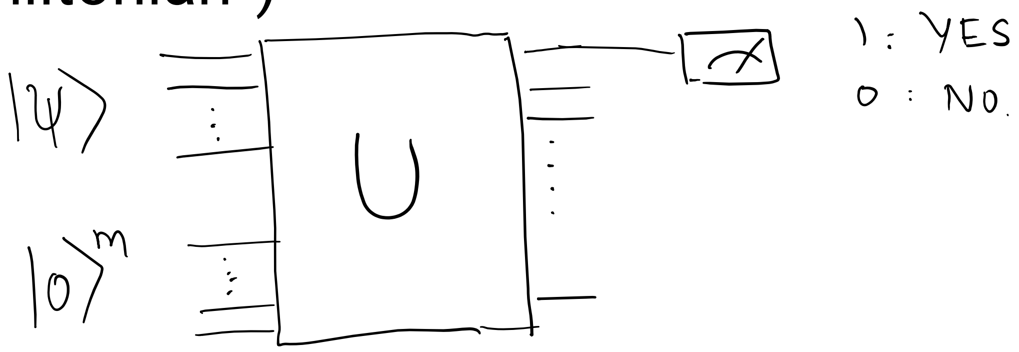
- GQMA$[c, s, d_1, d_2]$: QMA but with further promises
- Define $Q \ = |0\rangle^{\otimes m} \Pi_{\text{in}} U^* \, \Pi_{\text{out}} U \Pi_{\text{in}} \langle 0|^{\otimes m}$, operator on proof register
- Eigenvalues of Q $(\lambda_1 \geq \lambda_2 \geq \cdots)$ are accept probabilities of a complete basis of proof states

- If YES, $\lambda_1 \geq c$ and $\lambda_2 \leq \lambda_1 - d_1$
- If NO, $\lambda_1 \leq s$ and $\lambda_2 \leq \lambda_1 - d_2$
- Polynomially gapped QMA: PGQMA = $\cup_{c-s \geq 1/\text{poly}}$GQMA$[c, s, 1/\text{poly}, 1/\text{poly}]$

- Precise variant: PrecisePGQMA = $\cup_{c-s \geq 1/\text{exp}}$GQMA$[c, s, 1/\text{poly}, 1/\text{poly}]$

QMA-hardness of Local Hamiltonian

- i.e. If one can solve LocalHamiltonian in general, one can also solve *any* QMA problem
- Proof strategy: given a QMA protocol, convert it into a Hamiltonian such that its ground state energy encodes the answer ("reduce from QMA to LocalHamiltonian")



YES: $\exists |\psi\rangle$: $\Pr(1) \geq c$
NO: $\forall\, |\psi\rangle$: $\Pr(1) \leq s$

- Feynman's idea: construct a counter (clock), and look at the "clock Hamiltonian"

$$H = H_{\text{in}} + H_{\text{prop}} + H_{\text{out}} + H_{\text{clock}}$$

- Clock has states $|0\rangle, |1\rangle, |2\rangle, \ldots |T\rangle$ ($T = \text{poly}$ is the <u>size</u> of the circuit)

Clock construction

- $H_{\text{prop}} = -\sum_j U_j \otimes |j\rangle\langle j-1|_{\text{clock}} + \text{h.c.}$
- $H_{\text{in}} = \sum_i |1\rangle\langle 1|_i \otimes |0\rangle\langle 0|_{\text{clock}} + \sum_{j\neq 0} |j\rangle\langle j|_{\text{clock}}$ to penalise bad input
- H_{clock} to penalise bad clock states
- $H_{\text{out}} = |0\rangle\langle 0|_{\text{out}} \otimes |T\rangle\langle T|_{\text{clock}}$ to penalise computations giving "NO" at the end of the circuit

H has low-energy states if they are valid computations and have high probability of being accepted at output

- YES case: ground state energy $\leq \frac{1-c}{T+1}$
- NO case: ground state energy is always $\geq \frac{1-s}{2T^3}$

Small-penalty clock construction

- $H_{\text{prop}} = -\sum_j U_j \otimes |j\rangle\langle j-1|_{\text{clock}} + \text{h.c.}$
- $H_{\text{in}} = \sum_i |1\rangle\langle 1|_i \otimes |0\rangle\langle 0|_{\text{clock}} + \sum_{j\neq 0} |j\rangle\langle j|_{\text{clock}}$ to penalise bad input
- H_{clock} to penalise bad clock states
- $H_{\text{out}} = \varepsilon|0\rangle\langle 0|_{\text{out}} \otimes |T\rangle\langle T|_{\text{clock}}$ to penalise computations giving "NO" at the end of the circuit

Low-energy subspace is close to that of $H_{\text{prop}} + H_{\text{in}} + H_{\text{clock}} =: H_0$.

Ground space of H_0: $\text{span}\{\frac{1}{\sqrt{T+1}}\sum_i U_i \ldots U_1 U_0|0\rangle^{\otimes m}|\phi\rangle|i\rangle$, $|\phi\rangle$ arbitrary}

H_{out} is what creates the (spectral as well as promise) gaps

Small-penalty clock construction

- H_{out} adds frustration and breaks degeneracies according to accept probabilities
- Lowest-lying eigenvalues of H related to those of Q, up to $1/\text{poly}$ disturbances

- Perturbation theory/Schrieffer-Wolff to analyse low-energy states for $\varepsilon \ll$ spectral gap of H_0.
- Eigenvalues given by $\frac{\varepsilon}{T+1}(1-\lambda_i)+O(\varepsilon^2)$
- λ_i: Probability that ith eigenstate of Q is accepted at output

PP upper bound for PrecisePGQMA

- "Power method": if you take repeated powers of Q, behaviour is dominated by largest eigenvalue
- Spectral gap controls efficacy

$$Tr(Q^q) = \lambda_1^q \left(1 + \left(\frac{\lambda_2}{\lambda_1} \right)^q + \cdots \right) \leq \lambda_1^q + \lambda_1^q \left(1 - \left(\frac{\Delta}{\lambda_1} \right)^q \right) \times d$$

- In PP, can compute trace of polynomially large powers of Q (even for exponentially large Q, but other conditions exist)
- Write trace as path integral

PP lower bound for gapped Local Hamiltonian

- Use PP = PreciseBQP
- Clock Hamiltonian for regular quantum computation, i.e. without a witness
- Aharonov et al[1]. showed $1/\mathrm{poly}$ spectral gap for this Hamiltonian (to show that adiabatic quantum computing is universal)
- Use modified clock Hamiltonian: estimating energy more precisely can decide PreciseBQP (= PP)
- Proof that modified Hamiltonian also has spectral gap largely the same

[1] Aharonov et al., arXiv:quant-ph/0405098

PP lower bound for gapped Local Hamiltonian with classical description

- Use PP = PreciseBQP
- Clock Hamiltonian for regular quantum computation, i.e. without a witness
- Aharonov et al[1]. showed $1/\text{poly}$ spectral gap for this Hamiltonian (to show that adiabatic quantum computing is universal)
- Observation: one can classically describe a circuit to prepare a history state (since initial state is a classical bit-string).
- Same Hamiltonian and hence same spectral gap

[1] Aharonov et al., arXiv:quant-ph/0405098

Summary

Spectral gap (Δ)	(δ, Δ)-GS-Description-LocalHamiltonian		(δ, Δ)-LocalHamiltonian	
	$\delta = 1/\text{poly}$	$\delta = 1/\exp$	$\delta = 1/\text{poly}$	$\delta = 1/\exp$
$\Delta = 1/\text{poly}$	QCMA	PP	PGQMA	PP
$\Delta = 1/\exp$	QCMA	NP^PP	?	PSPACE
$\Delta = 0$	QCMA	NP^PP	QMA	PSPACE