

Computational Difficulty of Computing the Density of States

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We study the computational difficulty of computing the ground state degeneracy and the density of states for local Hamiltonians. We show that the difficulty of both problems is exactly captured by a class which we call $\#BQP$, which is the counting version of the quantum complexity class QMA . We show that $\#BQP$ is not harder than its classical counting counterpart $\#P$, which in turn implies that computing the ground state degeneracy or the density of states for classical Hamiltonians is just as hard as it is for quantum Hamiltonians.

Understanding the physical properties of correlated quantum many-body systems is a problem of central importance in condensed matter physics. The density of states, defined as the number of energy eigenstates per energy interval, plays a particularly crucial role in this endeavor. It is a key ingredient when deriving many thermodynamic properties from microscopic models, including specific heat capacity, thermal conductivity, band structure, and (near the Fermi energy) most electronic properties of metals. Computing the density of states can be a daunting task however, as it in principle involves diagonalizing a Hamiltonian acting on an exponentially large space, though other more efficient approaches which might take advantage of the structure of a given problem are not a priori ruled out.

In this work, we precisely quantify the difficulty of computing the density of states by using the powerful tools of quantum complexity theory. Quantum complexity aims at generalizing the well-established field of classical complexity theory to assess the difficulty of tasks related to quantum mechanical problems, concerning both the classical difficulty of simulating quantum systems as well as the fundamental limits to the power of quantum computers. In particular, quantum complexity theory has managed to explain the difficulty of computing ground state properties of quantum spin systems in various settings, such as two-dimensional lattices [1] and even one-dimensional chains [2], as well as fermionic systems [3].

We will determine the computational difficulty of two problems: First, computing the density of states of a local Hamiltonian, and second, counting the ground state degeneracy of a local gapped Hamiltonian. To this end, we will introduce the quantum counting class $\#BQP$ (sharp BQP), which constitutes the natural counting version of the class QMA (Quantum Merlin Arthur) which itself captures the difficulty of computing the ground state energy of a local Hamiltonian [4, 5]. Vaguely speaking, $\#BQP$ counts the number of possible “quantum solutions” to a quantum problem that can be verified using a quantum computer. We show that both problems, computing the density of states and counting the ground state degeneracy, are complete problems for the class $\#BQP$,

i.e., they are among the hardest problems in this class.

Having quantified the difficulty of computing the density of states and counting the number of ground states, we proceed to relate the complexity class $\#BQP$ to known classical counting complexity classes, and show the surprising result that $\#BQP$ equals $\#P$ (under weakly parsimonious reductions), where $\#P$ (sharp P) counts the number of possible solutions to a classical problem. Thus, counting solutions to quantum problems turns out to be no harder than counting solutions to classical problems. Phrased in terms of Hamiltonians, we show that computing the density of states and counting the ground state degeneracy of a classical spin system is just as hard as solving the same problem for a quantum Hamiltonian.

Quantum complexity classes.—Let us start by introducing the relevant complexity classes. The central role in the following is taken by the *verifier* V , which verifies “quantum solutions” (also called *proofs*) to a given problem. More formally, a verifier checking an n -qubit quantum proof (that is, a quantum state $|\psi\rangle$) consists of a $T = \text{poly}(n)$ length quantum circuit $U = U_T \cdots U_1$ (with local gates U_i) acting on $m = \text{poly}(n)$ qubits, which takes the n -qubit quantum state $|\psi\rangle_I$ as an input, together with $m - n$ initialized ancillas, $|0\rangle_A \equiv |0 \cdots 0\rangle_A$, applies U , and finally measures the first qubit in the $\{|0\rangle_1, |1\rangle_1\}$ basis to return 1 (“proof accepted”) or 0 (“proof rejected”). Then, the class QMA contains all problems of the form: “Decide whether there exists a $|\psi\rangle$ such that $p_{\text{acc}}(V(\psi)) > a$, or whether $p_{\text{acc}}(V(\psi)) < b$ for all $|\psi\rangle$, for some chosen $a - b > 1/\text{poly}(N)$, given that one is the case”. Here, the acceptance probability of a state $|\psi\rangle$ is $p_{\text{acc}}(V(\psi)) := \langle \psi | \Omega | \psi \rangle$, with

$$\Omega = (\mathbb{1}_I \otimes \langle 0 |_A) U^\dagger (|1\rangle\langle 1|_1 \otimes \mathbb{1}) U (\mathbb{1}_I \otimes |0\rangle_A), \quad (1)$$

which we illustrate in Fig. 1.

The idea behind this definition is that QMA quantifies the difficulty of computing the ground state energy $E_0(H)$ of a local Hamiltonian H up to $1/\text{poly}(n)$ accuracy. Let the verifier be a circuit estimating $\langle \psi | H | \psi \rangle$; then a black box solving QMA problems can be used to compute $E_0(H)$ up to $1/\text{poly}(n)$ accuracy by binary search using a single QMA query. Note also that QMA is

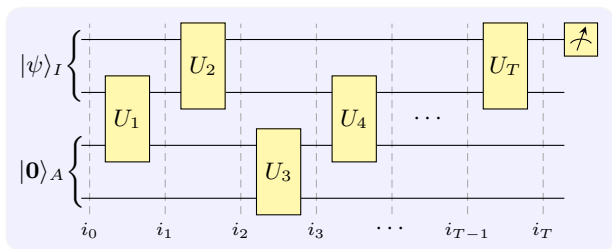


FIG. 1: A QMA verifier consists of a sequence of T local unitary gates acting on the “quantum proof” $|\psi\rangle$ and an ancillary register initialized to $|0\rangle$. The final measurement on the first qubit returns $|1\rangle$ or $|0\rangle$ to accept or reject the proof, respectively. Transition probabilities can be computed by doing a “path integral” over all intermediate configurations $(i_k)_k$.

the quantum version of the class NP, where one is given an efficiently computable boolean function $f(x) \in \{0, 1\}$ and one needs to figure out if there is an x such that $f(x) = 1$.

The class NP has a natural counting version, known as #P. Here, the task is to determine the *number* rather than the existence of satisfying inputs, i.e., to compute $\sum_x f(x) = |\{x : f(x) = 1\}|$. In the following, we will analogously define #BQP, the counting version of QMA. Consider the verifying map Ω of Eq. (1) for a QMA problem, with the additional promise that Ω does not have eigenvalues between a and b , $a - b > 1/\text{poly}(n)$. Then the class #BQP consists of all problems of the form “compute the dimension of the space spanned by all eigenvectors with eigenvalues $\geq a$ ” [17].

The promise we imposed on the spectrum of Ω is not present in the definition of QMA (though similarly restricted versions of QMA were defined in [6, 7]). Nevertheless, this promise emerges naturally when considering the counting version: QMA captures the difficulty of determining the existence of an input state with acceptance probability above a , up to a “grace interval” of $a - b$ in which mistakes are tolerated. Correspondingly, #BQP captures the difficulty of counting the number of (orthogonal) inputs with an acceptance probability above a , again with a “grace interval” of $a - b$ in which states are allowed to be miscounted. Similarly, the Hamiltonian formulation of the problem which we will discuss below asks for the existence (QMA) or number (#BQP) of states in a certain energy interval, where states which are in some small $1/\text{poly}(n)$ neighborhood of this interval may be miscounted.

The class #BQP inherits the important property from QMA of being stable under amplification, that is, the definition of #BQP is not sensitive to the choice of the gap $a - b$. In particular, any gap $a - b > 1/\text{poly}(n)$ can be efficiently amplified such that $a' = 1 - \exp(-\text{poly}(n))$, $b' = \exp(-\text{poly}(n))$ without changing the proof $|\psi\rangle$, by using a construction called *strong amplification*, which essentially repeatedly applies the verifier Ω and performs

majority voting. The construction can be found in [8], where it is also shown that the amplification acts on all eigenvectors independently. In particular, any state in the subspace with eigenvalues $\geq a$ can be amplified to have eigenvalues $\geq 1 - \exp(-\text{poly}(n))$, and any state in the other subspace to $\leq \exp(-\text{poly}(n))$. Using this amplification property, we will always choose a and b in the following as close to 1 and 0 as needed.

Complexity of computing density of states.—Let us now show why the class #BQP is relevant for physical applications. In particular, we are going to show that computing the density of states of a local n -spin Hamiltonian $H = \sum_i H_i$ with few-body terms H_i , up to accuracy $1/\text{poly}(n)$, is a problem which is complete for #BQP, i.e., it is as hard as any problem in #BQP can be. The same holds true for the (a priori weaker) problem of counting the ground state degeneracy of a local Hamiltonian, given a $1/\text{poly}(n)$ spectral gap above [18].

Let us start by defining the problems more precisely. The problem DOS (density of states) is the following: Given a local Hamiltonian $H = \sum_i H_i$, compute the number of orthogonal eigenstates with eigenvalues in an interval $[E_1, E_2]$ with $E_2 - E_1 > 1/\text{poly}(n)$, where states within a “grace interval” $\Delta = 1/\text{poly}(n) \ll E_2 - E_1$ around E_1 and E_2 can additionally be counted. Second, the problem #LH (sharp local Hamiltonian) corresponds to counting the number of ground states of a local Hamiltonian which has a spectral gap $\Delta = 1/\text{poly}(n)$ above the ground state subspace, and where we allow for an exponentially small splitting in the ground state energies.

Clearly, #LH is a special instance of DOS, i.e., solving #LH can be reduced to solving DOS. Let us now show that the problem DOS can be answered within the class #BQP: This is, we need to design a quantum circuit which accepts any input state $|\psi\rangle$ with an average energy $\langle \psi | H | \psi \rangle$ in the interval $[E_1, E_2]$ with high probability, while it also rejects any state with energy outside $[E_1 - \Delta, E_2 + \Delta]$ with high probability. This can be accomplished by using a phase estimation circuit [9], which maps any state $|\psi\rangle = \sum_i |\phi_i\rangle$ to $\sum_i |e_i + \delta_i\rangle |\phi_i\rangle$. Here, $|\phi_i\rangle$ are eigenstates of H_i with energy e_i , and $|\delta_i\rangle < \Delta/2$ is the error made by the phase estimation algorithm. By (coherently) setting the output qubit which signals acceptance of the input to 1 if and only if $E_1 - \Delta/2 \leq e_i + \delta_i \leq E_2 + \Delta/2$, we obtain a verifying circuit which has as many independent satisfying inputs as the original DOS Hamiltonian had eigenvalues in $[E_1, E_2]$, up to the grace interval Δ . This shows that any DOS problem can be reduced to solving a #BQP problem.

Let us now conversely show that #LH is a hard problem for #BQP, that is, any problem in #BQP can be reduced to counting the ground states of some gapped local Hamiltonian [19]. As in turn #LH can be reduced to DOS, which is contained in #BQP, this proves that both #LH and DOS are complete problems for the complexity class #BQP, i.e., they capture the full difficulty

of this class. To this end, we need to start from an arbitrary QMA verifier circuit $U = U_T \cdots U_1$ and construct a Hamiltonian which has as many ground states as the circuit has accepting inputs (corresponding to the outcome $|1\rangle_1$ on the first qubit). Since we can amplify QMA, we can assume that the acceptance and rejection probabilities are $a = 1 - \epsilon$ and $b = \epsilon$, with $\epsilon = \exp(-cn)$ for some $c > 1$. Let \mathcal{A} and \mathcal{R} be the eigenspaces of Ω [Eq. (1)] with eigenvalues $\geq a$ and $\leq b$, respectively. Let $U[\mathcal{A}] := \{U|\psi\rangle_I|\mathbf{0}\rangle_A : |\psi\rangle_I \in \mathcal{A}\}$, and note that for any $|\chi\rangle \in U[\mathcal{A}]$, $\langle \chi | (|1\rangle_1 \otimes \mathbb{1}) | \chi \rangle \geq a = 1 - \epsilon$.

We now follow Kitaev's original construction for a Hamiltonian encoding a QMA verifier circuit [4, 5], which for any proof $|\psi\rangle_I \in \mathcal{A}$ has the ‘‘proof history’’ $|\Phi\rangle = \sum_{t=0}^T U_t \cdots U_1 |\psi\rangle_I |\mathbf{0}\rangle_A |t\rangle_T$ as its ground state, where the third register is used as a clock. The Hamiltonian $H = H_{\text{init}} + \sum_{t=1}^T H_{\text{evol}}(t) + H_{\text{final}}$ has three types of terms: $H_{\text{init}} = \mathbb{1} \otimes (\mathbb{1} - |\mathbf{0}\rangle\langle\mathbf{0}|_A) \otimes |0\rangle\langle 0|_T$ makes sure the ancilla is initialized, $H_{\text{evol}}(t) = -U_t \otimes |t\rangle\langle t - 1|_T + \text{h.c.}$ ensures proper evolution from $t - 1$ to t , and $H_{\text{final}} = (\mathbb{1} - \Pi_{U[\mathcal{A}]}) \otimes |T\rangle\langle T|_T$ causes all states $|\Phi\rangle$ built from inputs $|\psi\rangle_I \in \mathcal{A}$ to be frustration-free ground states of H , while states from \mathcal{R} , or those with wrongly initialized ancillas or erroneous evolution, yield a higher energy. Note that we have chosen H_{final} different from the usual choice $H_{\text{final}}^{\text{std}} = |0\rangle\langle 0|_1 \otimes \mathbb{1} \otimes |T\rangle\langle T|_T$: This will simplify the analysis, and we will switch back to $H_{\text{final}}^{\text{std}}$ later on.

Why did we choose H_{final} the way we did? This way, H acts independently on the $T+1$ -dimensional subspaces spanned by $\{U_t \cdots U_1 |\psi\rangle_I |\mathbf{x}\rangle_A |t\rangle_T\}_{t=0, \dots, T}$ for any $|\psi\rangle \in \mathcal{A}$ or $|\psi\rangle \in \mathcal{R}$, and any basis $|\mathbf{x}\rangle_A$ of ancillas containing $|\mathbf{0}\rangle_A$. The restriction of H to any of these subspaces describes a random walk, with only two distinct cases: $|\psi\rangle_I \in \mathcal{R}$ and $|\mathbf{x}\rangle_A = |\mathbf{0}\rangle_A$, or otherwise. Each of these Hamiltonians can be easily shown to have a $1/\text{poly}(n)$ -spaced spectrum, and moreover, the ground state energy in the second case is $1/\text{poly}(n)$ above the first case: Thus, the total Hamiltonian H has a $1/\text{poly}(n)$ -spaced spectrum, and in particular a $1/\text{poly}(n)$ spectral gap above the ground state subspace. (A thorough discussion on this can be found in [10].) In order to recover $H_{\text{final}}^{\text{std}}$ (which is necessary as H_{final} is non-local), note that $H_{\text{final}}^{\text{std}} \geq H_{\text{final}} - \delta \mathbb{1}$ with $\delta = \sqrt{\epsilon}$, i.e., the energy of any excited state decreases by at most δ . On the other hand, the energy of any ‘‘good’’ history state built from $|\psi\rangle_I |\mathbf{0}\rangle_A$, $|\psi\rangle_I \in \mathcal{A}$, and thus of the ground state subspace, increases by at most ϵ , using the lower bound on the overlap of $U[\mathcal{R}]$ and $|0\rangle\langle 0|_1 \otimes \mathbb{1}$. Thus, we obtain a Hamiltonian which has a ground state subspace with splitting $\leq \exp(-cn)$, a $1/\text{poly}(n)$ spectral gap above it, and for which the dimension of the ground state subspace equals $\dim \mathcal{A}$, which proves #BQP-hardness of #LH [20].

While we have presented the proof that #LH is #BQP-hard for the case of the original Kitaev construction, in which the Hamiltonian has terms which are few-body but not spatially local, our argument applies equally to

other classes of Hamiltonians which have been shown to be QMA-complete. For instance, it also holds for one-dimensional chains with nearest-neighbor couplings [2], where the same argument as above can be applied, cf. [10]. On the other hand, it also holds for constructions which use so-called *perturbation gadgets* to obtain the Hamiltonian of the Kitaev construction given above in some order of perturbation theory, such as for nearest-neighbor Hamiltonians on a two-dimensional square lattice of qubits [1], since the spectrum changes at most as much as the neglected higher orders in the perturbation expansion, which are suppressed to order $1/\text{poly}(n)$. Note that this means that the ground state splitting can now be of order $1/\text{poly}(n)$; however, it can still be chosen to be polynomially smaller than the spectral gap.

Quantum vs. classical counting complexity.—As we have seen, the quantum counting class #BQP exactly captures the difficulty of counting the degeneracy of ground states and computing the density of states of local quantum Hamiltonians. In the following, we will relate #BQP to classical counting classes; in particular, we will prove that #BQP is equal to #P, counting the number of satisfying inputs to a boolean function [21]. In physical terms, this shows that counting the number of ground states or determining the density of states for a quantum Hamiltonian is not harder than either problem is for a classical Hamiltonian.

It is clear that #P is contained in #BQP: we can simply choose our quantum verifier to compute the value of the classical function encoding the #P problem. It remains to be shown that any #BQP problem can be solved by computing a #P function. We start from a verifier operator Ω , Eq. (1), and wish to show that the dimension of its accepting subspace, i.e., the subspace \mathcal{A} with eigenvalues $\geq a$, can be computed by counting satisfying inputs of some efficiently computable boolean function. To this end, we can again use strong amplification and choose $a = 1 - 2^{-(n+2)}$ and $b = 2^{-(n+2)}$. Then,

$$|\dim \mathcal{A} - \text{tr } \Omega| \leq 2^n 2^{-(n+2)} = \frac{1}{4},$$

i.e., we need to compute $\text{tr } \Omega$ to accuracy $\frac{1}{4}$. This can be done using a ‘‘path integral’’ method, which has been used previously to show containments of quantum classes in the classical classes PP and #P (see e.g. [11]). The idea is to rewrite $\text{tr } \Omega$ as a sum over products of transition probabilities along a path $\zeta \equiv (i_0, \dots, i_N, j_1, \dots, j_N)$, $\text{tr } \Omega = \sum_{\zeta} f(\zeta)$, where (see Fig. 1)

$$f(\zeta) = \langle i_0 |_I \langle \mathbf{0} |_A U_1^\dagger |j_1\rangle \langle j_1 | U_1^\dagger \cdots U_T^\dagger |j_T\rangle \times \langle i_T | [|0\rangle\langle 0|_1 \otimes \mathbb{1}] |i_T\rangle \langle i_T | U_T \cdots U_1 |i_0\rangle_I | \mathbf{0} \rangle_A. \quad (2)$$

Since any quantum circuit can be recast in terms of real gates U_t at the cost of doubling the number of qubits [12], $f(\zeta)$ can be assumed to be real. Computing $\sum_{\zeta} f(\zeta)$ to accuracy $\frac{1}{4}$ can now be easily mapped to summing over

a boolean function. First, in order to achieve the desired accuracy it is sufficient to approximate any f up to $|\zeta| + 2$ digits, where $|\zeta| = \text{poly}(n)$ is the number of bits in ζ . By letting $g(\zeta) := \text{round}[2^{|\zeta|+2}(f(\zeta) + 1)]$, we obtain a positive and integer-valued function $g(\zeta)$ satisfying $\left| [2^{-|\zeta|-2} \sum_{\zeta} g(\zeta) - 1] - \sum_{\zeta} f(\zeta) \right| \leq \frac{1}{4}$. Finally, we can write $g(\zeta) = \sum_{\xi \geq 0} h(\zeta, \xi)$ by defining a boolean indicator function $h(\zeta, \xi)$ which is 1 if $0 \leq \xi < g(\zeta)$, and 0 otherwise. This shows that $\text{tr } \Omega$ can be approximated to accuracy $\frac{1}{4}$, and thus $\dim \mathcal{A}$ can be determined by counting the number of satisfying assignments of a single boolean function $h(\zeta, \xi)$ that can be efficiently constructed from Ω , i.e., by a single query to a black box solving $\#P$ problems.

Summary and discussion.—In this work, we considered two problems: Computing the density of states and computing the ground state degeneracy of a local Hamiltonian of a spin system. In order to capture the computational difficulty of these problems we introduced the quantum complexity class $\#BQP$, the counting version of the class QMA. We proved that this complexity class exactly captures the difficulty of our two problems, even when restricting to local Hamiltonians on two-dimensional lattices of qubits or to one-dimensional chains, since all these problems are complete problems for the class $\#BQP$.

We have further shown that $\#BQP$ is no harder than its classical counterpart $\#P$. In particular this implies that computing the density of states is no harder for quantum Hamiltonians than it is for classical ones. While this quantum-classical equivalence is surprising at the Hamiltonian level, it should be noted that the classes $\#P$ and PP quite often form natural “upper bounds” for many quantum *and* classical problems.

What about the problem of computing the density of states for fermionic systems, such as many-electron systems? On the one hand, this problem will be still in $\#BQP$ and thus $\#P$, since any local fermionic Hamiltonian can be mapped via the Jordan-Wigner transform to a (non-local) Hamiltonian on a spin system, whose energy can still be estimated efficiently by a quantum circuit [13]. On the other hand, hardness of the problem for $\#BQP$ can be shown e.g. by using the $\#BQP$ -hardness of $\#LH$, and encoding each spin using one fermion in two modes, similar to [13]. Thus, computing the density of states for fermionic systems is a $\#BQP$ -complete problem as well.

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Note added.—After completion of this work, we learned that Shi and Zhang [14] have independently defined $\#BQP$ and have proved the same result on the relation of $\#P$ and $\#BQP$ using the same technique.

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 - [16] S. Bravyi, C. Moore, and A. Russell (2009), arXiv:0907.1297.
 - [17] An equivalent definition for $\#BQP$, cf. also [6, 7], is the following: Consider a verifier Ω with the additional promise that there exist subspaces $\mathcal{A} \oplus \mathcal{R} = \mathbb{C}^{2^n}$ such that $\langle \psi | \Omega | \psi \rangle \geq a$ for all $|\psi\rangle \in \mathcal{A}$, and $\langle \psi | \Omega | \psi \rangle \leq b$ for all $|\psi\rangle \in \mathcal{R}$, where again $a - b > 1/\text{poly}(n)$. Then $\#BQP$ consists of all problems of the form “compute $\dim \mathcal{A}$ ”. This is well-defined: For two decompositions $\mathcal{A} \oplus \mathcal{R}$ and $\mathcal{A}' \oplus \mathcal{R}'$, if w.l.o.g. $\dim \mathcal{A} > \dim \mathcal{A}'$, it follows $\dim \mathcal{A} + \dim \mathcal{R}' > 2^n$, and thus there exists a non-trivial $|\mu\rangle \in \mathcal{A} \cap \mathcal{R}'$, which is contradictory. This definition is also equivalent to our definition in terms of the spectrum of Ω : For one direction, let \mathcal{A} be spanned by the eigenvectors with eigenvalues $\geq a$, and for the other, one can use the minimax-principle for eigenvalues [15] to infer that Ω has a spectral gap between a and b , where the dimension of the eigenspace with eigenvalues $\geq a$ equals $\dim \mathcal{A}$.
 - [18] Indeed, it was suggested in Ref. [16] that computing the dimension of an eigenspace of a local Hamiltonian could directly provide a *definition* for what we call $\#BQP$.
 - [19] Note that the connection between QMA with a unique “good witness”, such as in our $\#BQP$ definition, and local Hamiltonians with unique ground state and a $1/\text{poly}(n)$ gap has been shown in [6].

- [20] In order to obtain an actual few-body Hamiltonian one needs to use a unary encoding of the clock, which however does not significantly change the low-energy spectral properties of the Hamiltonian [5].
- [21] Formally speaking, the reduction from $\#\text{BQP}$ to $\#\text{P}$ is *weakly parsimonious*, i.e., for any function $f \in \#\text{BQP}$ there exist polynomial-time computable functions α and β , and a function $g \in \#\text{P}$, such that $f = \alpha \circ g \circ \beta$. This differs from Karp reductions where no postprocessing is allowed, $\alpha = \text{Id}$, but it still only requires a single call to a $\#\text{P}$ oracle.