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for certain Satisfiability Problems

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We determine the complexity of several constraint satisfaction problems using the quantum adiabatic algorithm in its simplest implementation. We do so by studying the size dependence of the gap to the first excited state of "typical" instances. We find that at large sizes N, the complexity increases exponentially for all models that we study. We also compare our results against the complexity of the analogous classical algorithm WalkSAT and show that the harder the problem is for the classical algorithm the harder it is also for the quantum adiabatic algorithm.

I. INTRODUCTION

Theoretical research on quantum computing is motivated by the exciting possibility that quantum computers are inherently more efficient than classical computers due to the advantages that the laws of quantum mechanics provide, such as superposition, interference and entanglement. Besides the great effort of research towards the physical realization of these devices, a lot of activity has been devoted to the development of algorithms that could use quantum properties to achieve better efficiency in performing computational tasks with respect to classical devices.

Perhaps the best example to date for the superiority of quantum computers over classical ones is given by Shor's algorithm [1] for integer factorization, which solves the problem in polynomial time, whereas the best classical algorithm takes a time which is exponential in (a fractional power of) the problem size.

A rather general approach to solve a *broad range* of hard optimization problems using a quantum computer has been proposed by Farhi *et al.* [2]. Within the framework of this new approach, which was given the name the Quantum Adiabatic Algorithm (QAA), the solution to an optimization problem is encoded in the ground state of a Hamiltonian $\hat{H}_p$. To find the solution, the QAA prescribes the following course of action. As a first step, the system is prepared in the ground state of another Hamiltonian $\hat{H}_d$, commonly referred to as the driver Hamiltonian. The driver Hamiltonian is chosen such that it does not commute with the problem Hamiltonian and has a ground state which is fairly easy to prepare. As a next step, the Hamiltonian of the system is slowly modified from $\hat{H}_d$ to $\hat{H}_p$, using the linear interpolation, i.e.

$$\hat{H}(s) = s\hat{H}_p + (1-s)\hat{H}_d \,, \qquad (1)$$

where $s(t)$ is a parameter varying smoothly with time, from 0 at $t = 0$ to 1 at the end of the algorithm, $t = \mathcal{T}$. If this process is done slowly enough, the adiabatic theorem of Quantum Mechanics (see, e.g., Refs. [3] and [4]) ensures that the system will stay close to the ground state of the instantaneous Hamiltonian throughout the

evolution, so that one finally obtains a state close to the ground state of $\hat{H}_p$. At this point, measuring the state will give the solution of the original problem with high probability.

The running time $\mathcal{T}$ of the algorithm determines the efficiency, or complexity, of the QAA. An upper bound for the complexity can be given in terms of the eigenstates $\{|n\rangle\}$ and eigenvalues $\{E_n\}$ of the Hamiltonian, by [5, 6]

$$\mathcal{T} \gg \hbar \, \frac{|\max_s V_{10}(s)|}{(\Delta E_{\min})^2} \,, \qquad (2)$$

where $\Delta E_{\min}$ is the minimum of the first excitation gap $\Delta E_{\min} = \min_s \Delta E$ with $\Delta E = E_1 - E_0$, and $V_{n0} = \langle 0|\mathrm{d}\hat{H}/\mathrm{d}s|n\rangle$.

Typically, matrix elements of $\hat{H}$ scale as a low polynomial of the system size N, and the question of whether the complexity depends polynomially or exponentially with N therefore depends on how the minimum gap $\Delta E_{\min}$ scales with N. This means that if the gap becomes exponentially small at any point in the evolution, then the computation requires an exponential amount of time, rendering the QAA inefficient. The dependence of the minimum gap on the system size for a given problem is therefore a central issue in determining the complexity of the QAA.

The most interesting unknown about the QAA to date is thus whether or not it could solve in polynomial time "hard" sets of problems – those which belong to the NP-complete category [7] and for which all known algorithms take an exponential amount of time (exponential complexity) at least in the worst case. While early studies of the QAA done on very small systems ($N \leq 24$) [2, 8] provided some preliminary numerical evidence that the time required to solve one such NP-complete problem does scale only polynomially, roughly as N^2, several later studies gave evidence that this may not be the case.

Refs. [6, 9] show that adiabatic algorithms can fail if one does not choose the initial Hamiltonian carefully by taking into account the structure of the problem. Altshuler *et al.* [10] also argued that adiabatic quantum optimization will fail in general for random instances of NP-complete problems. However, the arguments of Altshuler *et al.* have been criticized by Knysh and Smelyanskiy [11].

In addition, Young *et al.* [12, 13] recently examined the 1-in-3 "constraint satisfaction", or SAT, problem (to be explained in the next section) and showed that very small gaps could appear in the spectrum of the Hamiltonian due to an avoided crossing between the ground state and another level corresponding to a local minimum of the optimization problem. This 'bottleneck' was shown to appear in a larger and larger fraction of the instances as the problem size N increases, indicating the existence of a first order quantum phase transition. This leads to an exponentially small gap of a *typical* instance, and therefore also to the failure of adiabatic quantum optimization. Other studies that considered this model have found an exponential complexity [14, 15] for *particularly hard* instances of small size.

It is not yet clear however to what extent the above behavior found for 1-in-3 SAT is general and whether it is a feature inherent to the QAA that will plague most if not all problems fed into the algorithm or something far more restricted than this. Previous work [16–18] had argued that a first order quantum phase transition occurs for a broad class of random optimization models. To gain further insight into this matter we study here three optimization problems which had previously been suggested [17, 19, 20] as good potential candidates for detailed investigation.

The problems we study are of the "constraint satisfaction" type. For these, one asks a questions for which there is a "yes" or "no" answer, namely whether there is an assignment of N bits which satisfies all of M logical conditions (clauses). An energy is assigned to each clause such that it is zero if the clause is satisfied and positive if it is not.

The first two problems we focus on in this paper are "locked" problems – a term first introduced by Zdeborová and Mézard [19, 20] for problems with instances having the following two properties: (i) every variable is in at least two clauses, and (ii) one can not get from one satisfying assignment to another by flipping a single bit. In fact, it was argued that typically order $\ln N$ bits needs to be flipped to go from one solution to another. These locked problems have several properties that make them eminently suitable as benchmarks. They are analytically "simple" (or at least simpler than previously studied models such as random K-SAT), but are computationally hard. Also, fluctuations between instances are smaller than with "unlocked" problems. Specifically, we study here the complexity of the QAA for the locked 1-in-3 SAT and locked 2-in-4 SAT models which belong to the NP-complete category.

In addition, we also compare our results with those of a third model, 3-regular 3-XORSAT, already considered by Jörg *et al.* [17], and Farhi *et al.* [21]. As we shall see, this model, while belonging to the P complexity class (i.e., it could be solved in polynomial time) is very hard to solve computationally by general purpose algorithms.

We study these models by analyzing the size dependence of the typical gap by means of quantum Monte Carlo (QMC) simulations. The plan of this paper is as follows: Section II describes the three models that will be studied. In Sec. III we discuss the manner in which we obtain our results. These results are presented in Sec. IV and our conclusions are summarized in Sec. V.

II. MODELS

We consider problems of the "constraint satisfaction" type, in which there are N bits (or equivalently, Ising spins) and M "clauses" where each clause is a logical condition on a small number of randomly chosen bits. A configuration of the bits (spins) is a "satisfying assignment" if it satisfies all the clauses.

In encoding this type of problem as a quantum Hamiltonian, each bit variable is represented in the Hamiltonian by the z-component of a Pauli matrix, σ_i^z, where i labels the spin. Each clause is thus converted to an energy function which depends on the spins associated with the clause, such that the energy is zero if the clause is satisfied and is positive (in our case, one) if it is not. The general structure of the problem Hamiltonian $\hat{H}_p$ is therefore

$$\hat{H}_p = \sum_{a=1}^{M} \hat{H}_a \,, \qquad (3)$$

where a is the clause index and $\hat{H}_a$ is the energy associated with the clause and involves the spins belonging to it.

Clearly, it is easy to satisfy all clauses if the ratio $\alpha \equiv M/N$ is small enough. In fact, one expects an exponentially large number of satisfying assignments in this region. Conversely, if M/N is very large, with high probability there will be a conflict between different clauses. Hence there is a "satisfiability transition" at some value α_s where the number of satisfying assignments goes to zero. It is particularly hard to solve satisfiability problems close to the transition [22], so we will work in this region.

Furthermore, when studying the efficiency of the QAA numerically [2, 12, 13], it is convenient to consider instances with a unique satisfying assignment (USA), which, of course, forces the system to be close to the transition. Considering instances with a USA is particularly advantageous for locked problems. While for unlocked problems the entropy of solutions at the satisfiability threshold is positive [23], for locked problems it approaches zero continuously [19, 20]. This means that while solutions with USA are rare for unlocked problems, they are expected to be among the 'typical' instances for locked problems and therefore locked problems have the advantage that instances with a USA should be a good representation of *randomly chosen* instances. Indeed, this is supported by a recent numerical study [24] that found that the probability of a USA only decreases

	locked 1-in-3	locked 2-in-4
N	M	M
16	13	11
24	–	17
32	25	23
40	–	28
48	38	34
64	51	–
96	76	–

TABLE I: Values of M and N for the locked instances.

slowly with N and appears to tend to a nonzero value as $N \to \infty$.

We now discuss the different models that will be investigated in this paper.

A. Locked 1-in-3 SAT

In the 1-in-3 SAT problem each clause consists of three bits chosen randomly, and the clause is satisfied if one of the bits is one and the others are zero. Here we fix the ratio M/N to be the critical value for the satisfiability transition. According to Table I of Ref. [20], this is equal to $\alpha_s = 0.789$. Since M has to be an integer we take M to be the nearest integer to $\alpha_s N$, see Table I. Note that, if the sites are chosen at random to form the clauses, the distribution of the degree of the sites (i.e., the number of clauses involving a site) would be Poissonian. However, locked instances have a minimum degree of two, so instead we use a truncated Poissonian distribution [20] which is Poissonian except that the probabilities for zero and one are set to zero.

We study instances with a unique satisfying assignment (USA). For these instances the gap to the first excited state is of order unity at $s = 1$ (and also of order unity at $s = 0$) so the gap has a minimum whose value is related to the complexity. For instances with many satisfying assignments the ground state of the problem Hamiltonian is degenerate and so the gap to the first excited state decreases to zero as $s \to 1$. Hence this gap would give no information about the computer time needed to determine whether there is a state with zero energy.

The energy of a clause for the locked 1-in-3 problem is given by:

$$\hat{H}_a = \frac{1}{8}\Big(5 - \sigma_{a_1}^z - \sigma_{a_2}^z - \sigma_{a_3}^z \qquad (4)$$
$$+ \sigma_{a_1}^z \sigma_{a_2}^z + \sigma_{a_2}^z \sigma_{a_3}^z + \sigma_{a_3}^z \sigma_{a_1}^z + 3\sigma_{a_1}^z \sigma_{a_2}^z \sigma_{a_3}^z \Big),$$

where a denotes the index of the clause and the a_i ($i = 1, 2, 3$) label the participating spins. With this Hamiltonian, the energy is zero if the clause is satisfied and is one otherwise.

B. Locked 2-in-4 SAT

We also consider locked 2-in-4 instances, in which a clause has four bits, and is satisfied if two are zero and two are one. Unlike the locked 1-in-3 SAT model discussed above, this model has a symmetry under flipping all the bits.

We fix the ratio M/N to be the critical value for the satisfiability transition. According to Table I of Ref. [20], this is equal to $\alpha_s = 0.707$. Again, since M has to be an integer we take M to be the nearest integer to $\alpha_s N$, see Table I.

In this problem, the energy of a clause is given by:

$$\hat{H}_a = \frac{1}{8}\Big(5 + \sigma_{a_1}^z \sigma_{a_2}^z + \sigma_{a_1}^z \sigma_{a_3}^z + \sigma_{a_1}^z \sigma_{a_4}^z + \sigma_{a_2}^z \sigma_{a_3}^z$$
$$+ \sigma_{a_2}^z \sigma_{a_4}^z + \sigma_{a_3}^z \sigma_{a_4}^z - 3\sigma_{a_1}^z \sigma_{a_2}^z \sigma_{a_3}^z \sigma_{a_4}^z \Big), \qquad (5)$$

where, as before, a denotes the index of the clause and the a_i ($i = 1, 2, 3, 4$) label the participating spins. For this energy term, a satisfied clause has zero energy and an unsatisfied one has energy one.

Because of bit-flip symmetry the energy of a state of the problem Hamiltonian is the same as that of the state obtained by flipping all the bits. Hence, when we refer to an instance with a "unique" satisfying assignment (USA) for the locked 2-in-4 problem, we will ignore states related by symmetry (so the true ground state degeneracy is actually two, not one).

C. 3-regular 3-XORSAT

Another problem we discuss here is the 3-regular 3-XORSAT problem, already considered by Jörg *et al.* [17] and Farhi *et al.* [21]. In the 3-XORSAT problem, three bits are chosen to form a clause and the clause is satisfied if their *sum* (mod 2) is a specified value (either 0 or 1). Alternatively, in terms of spins, the clause is satisfied if the *product* of the three σ_i^z's is a specified value (either -1 or 1).

We will consider here the "3-regular" case where every bit is in exactly three clauses, a model which turns out to be *precisely* at the satisfiability threshold. Note that this implies $M = N$. Again, the problem to be solved is whether there is an assignment of the bits which satisfies all the clauses. Interestingly, since this problem just involves linear algebra (mod 2), the satisfiability problem can be solved in polynomial time using, for example, Gaussian elimination. However, as is already well known (see, e.g., [25, 26]) and will also become evident soon, the problem is very hard for general purpose algorithms. Furthermore, if there is *no* satisfying assignment, no known polynomial time algorithm will determine the minimal number of unsatisfied clauses, a problem known as MAX-XORSAT.

As usual, we consider instances with a USA. Fortunately, these are *a nonzero fraction*, about 0.285 [17], of

the total, so the USA instances should be a good representation of randomly chosen ones. For XORSAT instances with a USA, it is not difficult to show that one can gauge transform any instance into one in which the sum of the bits of every clause is equal to 0 (mod 2). The USA is then all bits equal to 0, (a "ferromagnetic" ground state in statistical physics language). Although this ground state is "trivial", we shall see that it is very hard to find using general purpose algorithms including the QAA.

The energy of a clause in this model is:

$$\hat{H}_a = \frac{1}{2}\left(1 - \sigma^z_{a_1}\sigma^z_{a_2}\sigma^z_{a_3}\right) , \qquad (6)$$

where again a denotes the index of the clause and the a_i $(i = 1, 2, 3)$ label the participating spins.

D.   The driver Hamiltonian

Before moving on, we note that the driver Hamiltonian we choose here is perhaps the simplest possible choice,

$$\hat{H}_d = \frac{1}{2}\sum_i \left(1 - \sigma^x_i\right) , \qquad (7)$$

where σ^x_i is the x-component Pauli matrix acting on spin i. This corresponds to a transverse field of equal size on all sites. Its ground state is a uniform superposition of all 2^N states of the computational (i.e. σ^z) basis.

III.   METHOD

As was already mentioned, the complexity of the QAA algorithm is determined by the size dependence of the "typical" minimum gap of the problem. Following Refs. [12] and [13], we analyze the size-dependence of these gaps for each of the problems discussed in the previous section by considering typically 50 instances for each size, and then extracting the minimum gap for each of them. As a next step, we take the median value of the minimum gap among the different instances for a given size to obtain the "typical" minimum gap.

To find the minimum gap for a specific instance of a specific problem, we perform quantum Monte Carlo simulations for a range of s values that bracket the minimum gap. For each of the studied s values we extract the gap and interpolate the minimum value using a simple quadratic fit. An illustrative example of this is given in Fig. 1

In cases where we find that the mesh of s values is either too crude or does not bracket the minimum gap, a second round of simulations, with a more appropriate mesh of s values, is launched.
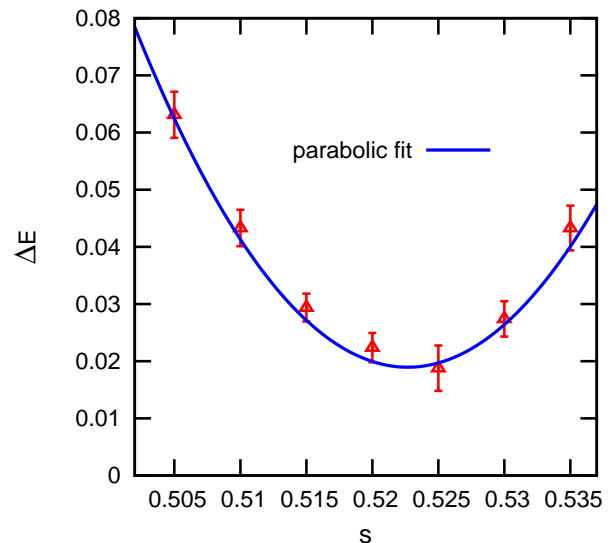

FIG. 1: (Color online) Gap to the first excited state as a function of s for one instance of the locked 1-in-3 SAT problem. The line is a quadratic fit to the data points from which the location, $s = 0.523$, and value, $\Delta E_{\min} = 0.207$, of the minimum gap are obtained. Here, $N = 64$ and $\beta = 1024$.

A.   The quantum Monte Carlo technique

To study the behavior of the typical minimum gap for large ($N > 24$) system sizes for which exact diagonalization routines are unfeasible, we employ a continuous-time quantum Monte Carlo technique. As the name indicates, this technique is based on sampling the 2^N states of the Hilbert space, so there are therefore statistical errors stemming from the nature of the procedure. However, Monte Carlo methods provide the only numerical method available for investigating large system sizes.

The specific method we use in this study is known as the stochastic series expansion (SSE) algorithm [27, 28] which involves a Taylor series expansion of the partition function $\mathrm{Tr}[e^{-\beta\hat{H}}]$ and uses a discrete representation of continuous imaginary time. This discretization however does not introduce errors into the algorithm as is the case in the alternative path-integral formulation, where one usually performs a Trotter-type discretization of imaginary time, see e.g. Refs. [12, 13], though formulations in continuous imaginary time also exist [29, 30]. Here β is the inverse temperature $1/T$ (in our units $k_B = 1$).

The SSE algorithm has several properties that are very useful in addressing the problems we focus on in this study. Firstly, it works in continuous imaginary time as discussed above. Secondly, it allows not only local updates of system configurations but also global cluster updates, which in most cases prove to be more efficient than single-spin-flip updates. These global updates are achieved by dividing the configurations of the system produced by the QMC into clusters and then flipping a fraction of them within each sweep of the simulation [31]. An important bonus of cluster updates is the ex-

istence of "improved estimators" for determining time-dependent correlation functions, for which the signal to noise is much better than with conventional measurements.

In addition, we speed up equilibration by implementing "parallel tempering" [32], where simulations for different values of s are run in parallel and spin configurations with adjacent values of s are swapped with a probability satisfying the detailed balance condition. Traditionally, parallel tempering is performed for systems at different temperatures, but here the parameter s plays the role of (inverse) temperature.

We extract the gap from imaginary time-dependent correlation functions. However, in the locked 2-in-4 case, where the problem has bit-flip symmetry, this is tricky using the standard SSE algorithm and, as discussed next, we will use a different approach.

The difficulty arises for the following reason. Eigenstates of the Hamiltonian are either even or odd under bit-flip symmetry (in particular, the ground state is even). In the $s \to 1$ limit, states occur in even-odd pairs with an exponentially small gap (see Fig. 2 for an illustration). Therefore, the quantity of interest is the gap to the first *even* state. We consider correlation functions of even quantities, so there are only matrix elements between states of the same parity. However, the lowest odd level becomes very close to the ground state near where the gap to the first even excited state has a minimum, see Fig. 2. Hence this lowest odd state becomes thermally populated, with the result that odd-odd gaps are present in the data as well.

We have eliminated these undesired contributions by projecting out the symmetric subspace of the Hamiltonian. A way of doing this projection at zero temperature was proposed independently by Eddie Farhi [33] and Anders Sandvik [34]. In standard quantum Monte Carlo simulations one imposes *periodic* boundary conditions in imaginary time τ at $\tau = 0$ and β. To project out the symmetric subspace one imposes, instead, *free* boundary conditions [35] at $\tau = 0$ and β. The properties of the symmetric subspace can then be obtained, for $\beta \to \infty$, by measurements far from the boundaries. We have incorporated this idea into the SSE scheme, and use this modified algorithm in the simulations of the locked 2-in-4 problem.

To verify that our implementations of the SSE methods are accurate, we have compared their results with corresponding exact diagonalization results on small system sizes. The results agree within the error bars. A comparison of the gap is shown in Fig. 2. The careful will reader note that the QMC data is slightly but consistently above the diagonalization results. This is due to contributions from higher excited states at short times which increase the value of the time-dependent correlation function used to extract the gap in this limit, see Fig. 2 and Sec. III B. The effect is small even for the $N = 16$ data shown in Fig. 2, and we expect it to be smaller still for larger sizes near the minimum gap, since the gap is smaller so there
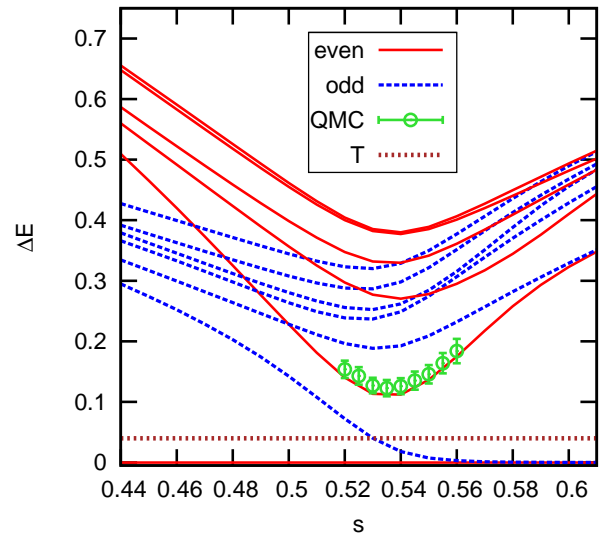

FIG. 2: (Color online) Energy gaps to even (solid, red) and odd (dashed, blue) excited states for an $N = 16$ instance of the locked 2-in-4 problem, which has bit-flip symmetry as discussed in the text. The dotted line shows a characteristic value of another important energy scale in the problem, temperature. In the region where the gap to the first even state has a minimum, the gap to the first odd state becomes very small and is inevitably thermally populated. Hence, odd-odd gaps appear in this region as well as even-even gaps. This is the reason why we use a non-standard Monte Carlo algorithm for this problem which projects out the symmetric subspace, so only even-even gaps are present in the data. The figure also shows the gap obtained from the even-subspace projected QMC in vicinity of the minimum. It agrees with exact diagonalization within the error bars.

is a larger region with straight-line behavior in plots like Fig. 3.

B. Extraction of the system gap

The gap of the system for a given instance and a given s value is extracted by analyzing measurements of (imaginary) time-dependent correlation functions of the type

$$C_A(\tau) = \langle \hat{A}(\tau)\hat{A}(0)\rangle - \langle A\rangle^2 \,, \tag{8}$$

where the operator $\hat{A}$ is some measurable physical quantity. In practice, we found it useful to construct superpositions of such correlation functions. Typically we use linear combinations of correlation functions of the operators σ_i^z or $\sigma_i^z \sigma_j^z$ where i and j run from 1 to N and label the spins. The evaluation of $\langle A\rangle^2$ in the above equation is computed from the product $\langle A\rangle^{(1)}\langle A\rangle^{(2)}$ where the two indices correspond to different independent simulations of the same system. This eliminates the bias stemming from straightforward squaring of the expectation value.

In the low temperature limit, $\Delta E \ll T$ where $\Delta E = E_1 - E_0$, the system is in its ground state so the
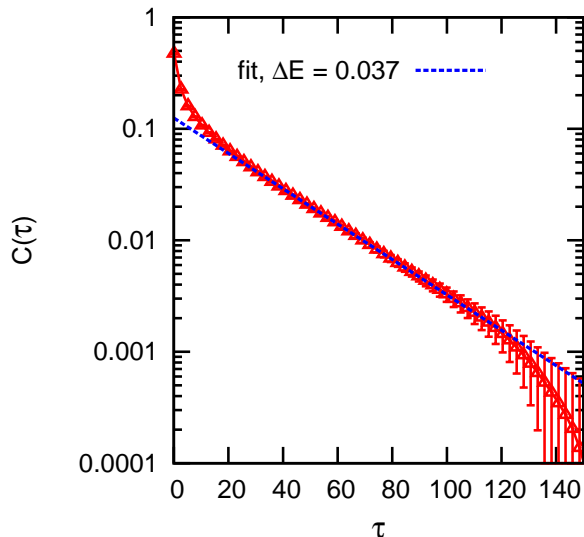
FIG. 3: (Color online) A log-linear plot of a time dependent correlation function for an instance of the locked 1-in-3 SAT problem with $N = 64$ spins, $\beta = 1024$, near the minimum gap at $s = 0.54$. The energy gap is the negative of the slope at large values of imaginary-time τ. A fit gives $\Delta E = 0.037$.

imaginary-time correlation function is given by

$$C_A(\tau) = \sum_{m=1} |\langle 0|\hat{A}|m\rangle|^2 \left(e^{-\Delta E_m \tau} + e^{-\Delta E_m (\beta - \tau)} \right) , \quad (9)$$

where $\Delta E_m = E_m - E_0$. At long times, τ, the correlation function is dominated by the smallest gap, $\Delta E \equiv \Delta E_1$, (as long as the matrix element $|\langle 0|\hat{A}|1\rangle|^2$ is nonzero). On a log-linear plot $C_A(\tau)$ then has a region where it is a straight line whose slope is the negative of the gap. This can therefore be easily extracted by simple linear fitting.

An illustration of the above procedure is depicted in Fig. 3 showing one of the correlation functions measured and analyzed for the locked 1-in-3 problem for $N = 64$, $\beta = 1024$ and $s = 0.54$. The gap in this case is $\Delta E = 0.037$.

IV. RESULTS

A. Results from the QAA

We show results for the median minimum gap as a function of size for the locked 1-in-3 problem in Fig. 4 (log-lin) and Fig. 5 (log-log). A straight line fit works very well for the log-lin plot (goodness of fit parameter $Q = 0.26$) but very poorly for the log-log plot ($Q = 3.8 \times 10^{-12}$). This provides strong evidence that the minimum gap is exponentially small in the system size, and so the complexity of the QAA (at least in the simplest version considered here) is exponentially large in the system size.

The corresponding results for the locked 2-in-4 problem are shown in Fig. 6 (log-lin) and Fig. 7 (log-log). A
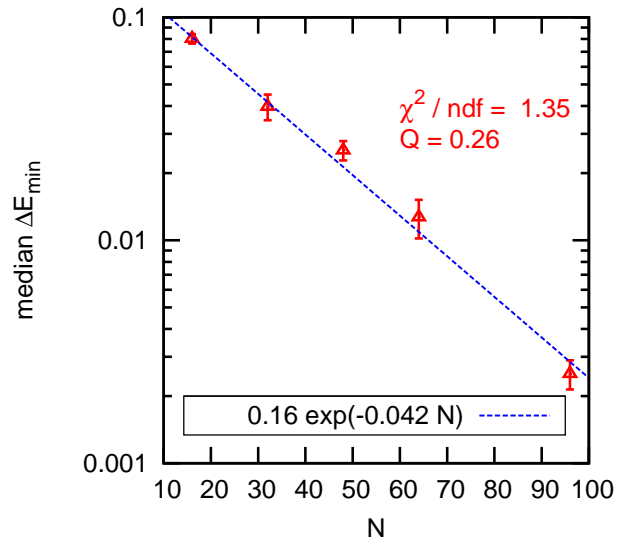

FIG. 4: (Color online) Median minimum gap on a log-linear scale for the locked 1-in-3 problem. The straight-line fit is good indicating the exponential complexity of the QAA for this problem.
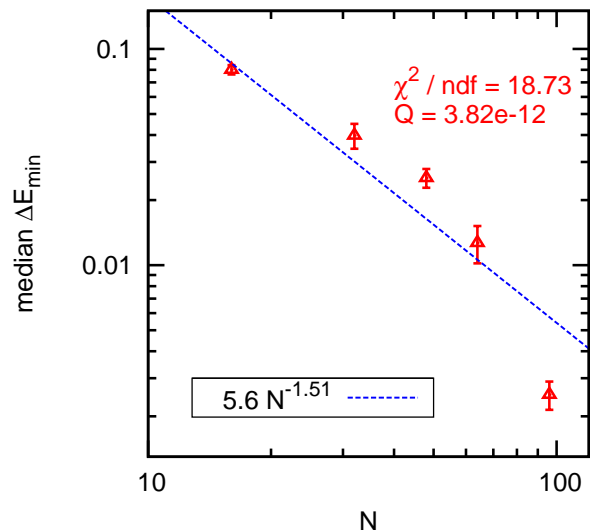

FIG. 5: (Color online) Median minimum gap on a log-log scale for the locked 1-in-3 problem. The straight-line fit is extremely poor indicating that the minimum gap for this problem is not polynomial in the system size.

straight line fit works very well for the log-lin plot ($Q = 0.19$) but poorly for the log-log plot ($Q = 5.9 \times 10^{-4}$). This provides strong evidence that the minimum gap is exponentially small in the system size.

The 3-regular 3-XORSAT problem has been studied by Jörg et al. [17] who determined the minimum gap for sizes up to $N = 24$ by diagonalization, and Farhi et al. [21] who extended the range of sizes up to $N = 40$ by quantum Monte Carlo simulations. The two sets of results agree and provide compelling evidence for an exponential minimum gap. Below we will compare the
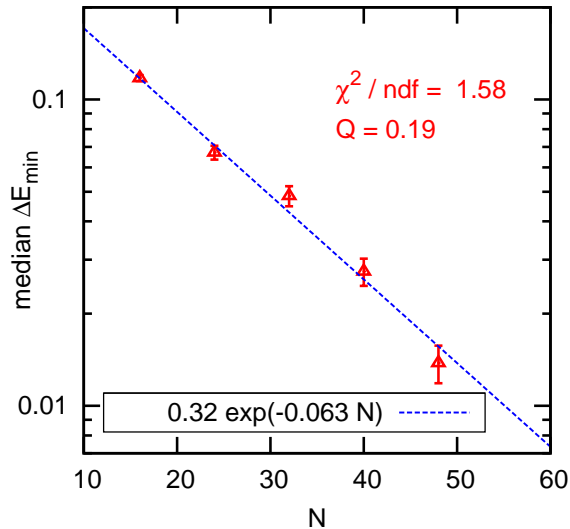
FIG. 6: (Color online) Median gap on a log-linear scale for the locked 2-in-4 problem. The straight-line fit is good indicating the exponential complexity for this problem.
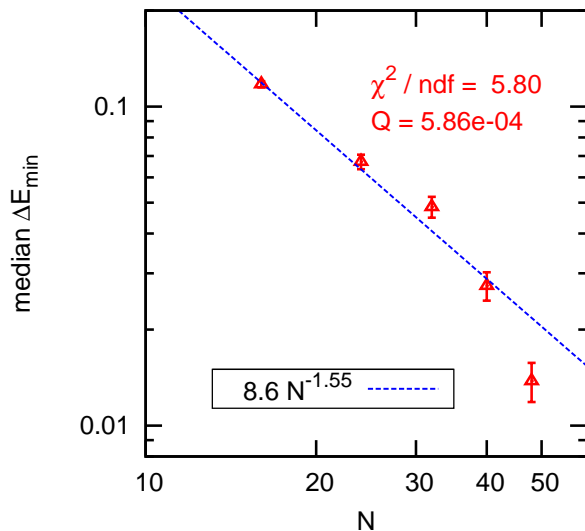

FIG. 7: (Color online) Median gap on a log-log scale for the locked 2-in-4 problem. The straight-line fit is poor indicating that the complexity for this problem is not polynomial.

coefficient in the exponent found by Jörg *et al.* and Farhi *et al.* with that for the other models studied here and with results from a *classical* algorithm.

B. Comparison with a classical algorithm

Since the QAA is designed to serve as an efficient tool for solving hard optimization problems it is interesting to compare its efficiency with that of a classical algorithm.

In Ref. [24] it was argued that a reasonable classical algorithm to compare with QAA is the heuristic local

model	μ(QAA)	μ(WalkSAT)	Ratio
locked 1-in-3 SAT	0.084(3) (this work)	0.0505(5) [24]	1.66
locked 2-in-4 SAT	0.126(5) (this work)	0.0858(8) [24]	1.47
3-reg 3-XORSAT	0.159(2) [21]	0.1198(20) [24]	1.32

TABLE II: Values of μ, the coefficient of N in the exponential complexity of the Quantum Adiabatic Algorithm (QAA), Eq. (10), versus that of the analogous classical algorithm WalkSAT, Eq. (11), and the ratios between them, for the three problems studied here. The data is taken from the references shown.

search algorithm known as WalkSAT [36], which is similar in spirit to simulated annealing in that both make moves which reduce the "energy", but also sometimes make moves which increase it to avoid being trapped in the nearest local minimum.

As discussed in Sec. I, Landau-Zener theory states that, for the QAA, the computation time is proportional to $1/\Delta E_{\min}^2$ (neglecting N dependence of matrix elements) and since we find that $\Delta E_{\min} \sim e^{-cN}$, the complexity can be written as

$$\mathcal{T} \propto e^{\mu N}, \tag{10}$$

where $\mu = 2c$.

In the WalkSAT algorithm, the running time is proportional to the number of "bit flips" the algorithm makes (for more details, the reader is referred to Ref [24]). Writing the median number of flips as

$$N_{\text{flips}} \propto e^{\mu N}, \tag{11}$$

we can now compare the exponent coefficients of the QAA versus those of WalkSAT. The latter were measured in Ref. [24]. For the convenience of the reader, the values of μ for both the QAA and WalkSAT are summarized in Table II.

As the table indicates, the exponent coefficients obtained with WalkSAT are somewhat smaller than those of the QAA, suggesting that the latter algorithm, in the specific way it was implemented in this paper, is slightly less efficient than its corresponding classical one for these three problems, although a problem-by-problem comparison shows that the coefficients are fairly similar. It is also evident from the table that the harder the problem is for WalkSAT, the harder it also is for QAA.

V. SUMMARY AND CONCLUSIONS

Using Quantum Monte Carlo (QMC) simulations, we studied the complexity of the Quantum Adiabatic Algorithm (QAA) for three constraint satisfaction problems, two of them in the NP complexity class – locked 1-in-3 SAT and locked 2-in-4 SAT – and one in the P complexity class – 3-regular 3-XORSAT. All three problems show exponential complexity (albeit with somewhat different coefficients), i.e. the computation time required by

the QAA to reach the solution of the problem Hamiltonian with high probability increases exponentially with the system size N.

We have also compared the QAA complexities against these of an analogous classical algorithm, WalkSAT and show the results in Table II. Perhaps not surprisingly we find that the harder the problem is for WalkSAT, the harder it also is for the QAA. Moreover, it seems that the coefficients of N in the exponential in the expression for the complexity of the QAA, Eq. (10), are somewhat larger than those of WalkSAT, Eq. (11) (with ratios ranging between about 1.3 and 1.7).

Several interesting questions arise upon examining the results of this study, and which we believe would be interesting to study in future work. The first one has to do with the possibility of avoiding the exponentially small gap by repeatedly running the algorithm with different random values for the transverse fields (and clause costs) [29]. It would also be interesting to look, more generally, for better paths in Hamiltonian space, perhaps by adding additional terms in the Hamiltonian for intermediate values of s, which would increase the minimum gap. In particular, can we find a clever way to optimize the path in Hamiltonian space "on the fly" during the simulation?

While the study reported here used instances with a unique satisfying assignment (USA), in which case the gap to the first excited state has a minimum which is related to the complexity, it would be interesting to also consider *random* instances to see if those too have exponential complexity in QAA. However this is numerically more challenging.

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[35] Free boundary conditions in the time direction are used in the path integral ground state (PIGS) Monte Carlo method, see e.g. Ref. [37], though its capability to project out states of a particular symmetry does not seem to have been emphasized. Similar ideas can also be used to

project out states with other attributes, see for example Refs. [38] and [39] in which states of a particular *total spin* are projected out.

[36] For information about WALKSAT see `http://www.cs.rochester.edu/~kautz/walksat/`.

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