Adiabatic quantum algorithms as quantum phase transitions: 1\textsuperscript{st} versus 2\textsuperscript{nd} order

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In the continuum limit (large number of qubits), adiabatic quantum algorithms display a remarkable similarity to sweeps through quantum phase transitions. We find that transitions of second or higher order are advantageous in comparison to those of first order. With this insight, we propose a novel adiabatic quantum algorithm for the solution of 3-satisfiability (3-SAT) problems (exact cover), which is significantly faster than previous proposals according to numerical simulations (up to 20 qubits). These findings suggest that adiabatic quantum algorithms can solve NP-complete problems such as 3-SAT much faster than the Grover search routine (yielding a quadratic enhancement), possibly even with an exponential speed-up.

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The realization that quantum algorithms (e.g., \cite{Grover1996, Farhi1998}) can solve certain problems much faster than (known) classical methods is one of the main motivations for constructing scalable quantum computers. Unfortunately, these efforts are strongly hampered by the decoherence induced by the inevitable coupling to the environment, which tends to destroy the fragile quantum features needed for these quantum algorithms. One idea to overcome this obstacle is adiabatic quantum computation\textsuperscript{2}, where the solution to the problem to be solved is encoded in the ground state of a suitably designed Hamiltonian $H_{\text{out}}$. In order to reach this (unknown) ground state, adiabatic quantum algorithms exploit the adiabatic theorem: A system described by a time-dependent Hamiltonian $H(t)$ with $H(t)|\Psi_n(t)\rangle = E_n(t)|\Psi_n(t)\rangle$ initially prepared in its ground state $|\Psi_0\rangle$ will approximately stay in its (instantaneous) ground state – provided the evolution of $H(t)$ is slow enough $\langle \Psi_0 | \dot{H} | \Psi_n \rangle \ll (E_n - E_0)^2$. Starting with an initial Hamiltonian $H_{\text{in}}$ whose ground state is known and easy to prepare, a sufficiently slow evolution into $H_{\text{out}}$, for example

$$H(t) = [1 - g(t)]H_{\text{in}} + g(t)H_{\text{out}},$$

where the parameter $g(t)$ runs from 0 to 1, generates the desired final ground state. With a sufficiently cold and weakly coupled environment, the occupation of the instantaneous ground state should be more robust against the impact of decoherence, see, e.g., \cite{Farhi1998}. The adiabatic condition $\langle \Psi_0 | \dot{H} | \Psi_n \rangle \ll (E_n - E_0)^2$ relates spectral properties of $H(t)$ with the runtime $T$ necessary to obtain a desired probability of the instantaneous ground state – which can be interpreted as the algorithmic complexity of the quantum algorithm. However, especially for NP-complete problems such as 3-SAT, the maximum speed-up achievable by adiabatic quantum algorithms is still not completely clear, see, e.g., \cite{Farhi1998, Schützhold2005, Schützhold2006, Schützhold2007}. In this Letter, we exploit the analogy to quantum phase transitions\textsuperscript{3} in order to gain new insight into these questions.

Let us start with one of the simplest examples: the Grover algorithm, which accomplishes the task to find a marked item in an unsorted database with $N = 2^n$ items with a quadratic speed-up\textsuperscript{2}. An adiabatic version of Grover’s algorithm is defined by the Hamiltonian

$$H(g) = (1 - g) [1 - |s\rangle \langle s|] + g [1 - |w\rangle \langle w|],$$

where $|s\rangle = \sum_{x=0}^{N-1} |x\rangle / \sqrt{N}$ denoting the superposition of all numbers from 0 to $N - 1$ and $|w\rangle$ the marked state, respectively. Since in this case the commutator between initial and final Hamiltonians $[H_{\text{in}}, H_{\text{out}}]$ is small, one can nearly diagonalize them simultaneously and the $g$-dependent spectrum will consist of nearly straight lines – except near $g_c = 1/2$, where we have an avoided level crossing, see Fig. 1. In the (continuum) limit of $n \rightarrow \infty$, this corresponds to a first-order quantum phase transition from $|s\rangle = |\rightarrow \rightarrow \rightarrow\rangle$ to $|w\rangle = |\uparrow\downarrow\uparrow\downarrow\rangle$ at the critical value $g_c = 1/2$. Such a first-order transition is characterized by an abrupt change of the ground state $|s\rangle$ for $g < g_c$ and $|w\rangle$ for $g > g_c$ resulting in a discontinuity of a corresponding order parameter such as $\langle \psi(g) | dH/dg | \psi(g) \rangle = dE/dg$.

Typically, quantum phase transitions of first order are associated with a $g$-dependent energy landscape sketched in Fig. 2, where the two competing ground states are separated by an energy barrier. During the phase transition, the system has to tunnel through that barrier between $|s\rangle$ and $|w\rangle$ in order to stay in the ground state. Since naturally the strength of this barrier increases with the system size $n$, one would expect the tunneling time to

\begin{figure}[ht]
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{Sketch of the level structure (ground state and first excited state) of the Grover Hamiltonian in Eq. (2).}
\end{figure}
qubits according to \( \sigma \) degree rotation around the qubit. This Hamiltonian is invariant under a global 180-

ground state is unique another simple model Hamiltonian and second order transitions a bit more), let us consider (and in order to bring out the difference between first 

tree for a second-order transition. As a counter-example behaves as scale exponentially – and indeed, the optimal runtime 

minimum gap behaves as ground state) scales polynomially in this case since the – and indeed, the optimal runtime (needed to stay in the 

tial to the final ground state much easier in this situation expect that the system should find its way from the ini-

transition with the black dot indicating the ground state.

FIG. 2: Sketch of the energy landscape for a first-order tran-

sition – the quantum Ising model in the presence of a transverse field as defined by the Hamiltonian

\[
H(g) = -(1 - g) \sum_{\alpha=1}^{n} \sigma^x_{\alpha} - g \sum_{\alpha=1}^{n} \sigma^z_{\alpha} \sigma^z_{\alpha+1},
\]

where \( \sigma^x, \sigma^z \) denote the Pauli matrices acting on the \( \alpha \)th qubit. This Hamiltonian is invariant under a global 180-degree rotation around the \( x \)-axis which transforms all qubits according to \( \sigma^z_{\alpha} \rightarrow -\sigma^z_{\alpha} \). The initial \( (g = 0) \) ground state is unique \( |s\rangle = |\cdots \rangle \), whereas the fi-

nal ground state \( (g = 1) \) becomes two-fold degenerate \( |w_1\rangle = |\cdots \uparrow \rangle, |w_2\rangle = |\cdots \downarrow \rangle \), and thereby breaks this symmetry. Typically, such a symmetry-breaking (or restoring) change of the ground state corresponds to a second-order phase transition. For the Ising model, this expectation can be confirmed analytically by an exact diagonalization of the Hamiltonian via Jordan-Wigner and Bogoliubov transformations (cf. [8, 10]). For such a second-order phase transition, the ground state changes continuously (i.e., there is no jump in an order parameter) and the energy barrier observed in first-order tran-

sitions is absent, see Fig. 3. Consequently, one would 

expect that the system should find its way from the ini-

tial to the final ground state much easier in this situation – and indeed, the optimal runtime (needed to stay in the 

ground state) scales polynomially in this case since the minimum gap behaves as \( O(1/n) \), cf. [8, 10]. 

Note, however, that symmetry-breaking is no guaran-

tee for a second-order transition. As a counter-example 

(and in order to bring out the difference between first 

and second order transitions a bit more), let us consider another simple model Hamiltonian

\[
H(g) = (1 - g)(1 - |s\rangle \langle s|) - g \sum_{\alpha=1}^{n} \sigma^x_{\alpha} \sigma^x_{\alpha+1},
\]

which combines the initial Hamiltonian of the Grover problem with the final Hamiltonian of the Ising model.

Even though it has the same symmetry and the same ini-

tial and final ground states as the Ising model, the above Hamiltonian leads to an avoided level crossing corre-

sponding to a first-order transition (as can be seen from the local geometry of the spectrum, data not shown [11]). 

As one would expect from the existence of the energy barrier in a first-order transition, cf. Fig. 2, the scaling of the runtime is exponential in this situation [6]. The main difference between the Ising model and the Hamiltonian above is that the latter choice involves \( n \)-qubit interactions \( |s\rangle = \prod_{\alpha=1}^{n} (1 + \sigma^x_{\alpha})/2 \) and therefore the bit structures of the initial and the final Hamiltonians are very different. These findings may shed additional light onto the recent discussions in Refs. [6, 12]. 

After having motivated the advantages of second-order phase transitions for adiabatic quantum computation, let 

us try to apply these findings to the solution of non-trivial computational problems. In order to compare our results to the literature, we are going to discuss a (well studied) special case of a 3-satisfiability problem: exact cover-3. 

This problem can be described as follows: a string of \( n \) bits \( z_{\alpha} \in \{0, 1\} \) must satisfy \( m \) constraints called clauses. Each clause involves three bits \( \alpha, \beta, \gamma \in \{1, \ldots, n\} \) and

\[
z_\alpha + z_\beta + z_\gamma = 1
\]

is the constraint to be satisfied for every triple \( (\alpha, \beta, \gamma) \). Evidently, the solution to this problem, i.e., the bit string satisfying all \( m \) constraints, is easy to verify but possibly hard to find – i.e., it belongs to the class NP. It can even be shown that exact cover-3 is NP-complete, i.e., all other NP-problems (such as factoring or the traveling salesman problem) can be mapped onto exact cover-3 with polynomial overhead. Of course, in order to study the speed-up of quantum algorithms in comparison with
classical methods, we are mostly interested in hard instances of this class of problems. First of all, it is believed that problems with a unique solution are among the hardest instances of exact cover-3. A further indication of the complexity can be obtained by treating the $m$ constraints of the form given by Eq. \ref{eq:3} as a system of linear equations. Clearly, for $m = n$ linearly independent constraints, the solution can be found easily. This suggests that instances with a small number of clauses – which still possess a unique solution – are particularly hard to solve, see also \ref{fig:1}. We shall consider both cases in the following and compare them.

In previous approaches (see, e.g., \ref{fig:3}), the Hamiltonian $H_{\text{out}}$ whose ground state encodes the solution to the aforementioned problem was constructed by assigning a fixed energy penalty to each violated clause. In contrast to this conventional choice (which involves three-qubit interactions) we shall use an alternative representation requiring two-qubit interactions only. (In view of an experimental setup, two-qubit interactions are probably favorably.) To this end, we sum the terms $(\sigma^z_\alpha + \sigma^z_\beta + \sigma^z_\gamma - 1)^2/4$ over all clauses $(\alpha, \beta, \gamma)$ and obtain \ref{eq:4}

$$H_{\text{out}} = \frac{1}{4} \sum_{\alpha, \beta = 1}^{n} M_{\alpha \beta} \sigma^z_\alpha \sigma^z_\beta - \frac{1}{2} \sum_{\alpha = 1}^{n} N_\alpha \sigma^z_\alpha , \quad (6)$$

plus an irrelevant constant. Here $N_\alpha$ denotes the number of clauses involving the bit $\alpha$ and $M_{\alpha \beta}$ is the number of clauses involving both bits $\alpha$ and $\beta$. The above Hamiltonian corresponds to a frustrated anti-ferromagnet in an external field, except that the interaction topology $M_{\alpha \beta}$ is defined by the clauses and not by physical neighborhood. For satisfiable problems, it has the same ground state (the solution) as the Hamiltonian used in \ref{fig:3}, but some of the excitation energies differ.

As we have seen in the example of Eq. \ref{eq:3}, the order of the phase transition crucially depends on the initial Hamiltonian. Therefore, the remaining task is to find a suitable initial Hamiltonian which respects the bit structure of the final Hamiltonian in Eq. \ref{eq:4} and whose ground state breaks a global symmetry – which hopefully generates a second-order transition. The symmetry of the final Hamiltonian we exploit here is its invariance under rotations around the $\Sigma_z$-axis, where

$$\Sigma^z = \sum_{\alpha = 1}^{n} \sigma^z_\alpha . \quad (7)$$

An initial Hamiltonian in which this symmetry is spontaneously broken is the Heisenberg ferromagnet

$$H_{\text{in}} = -\frac{1}{4} \sum_{\alpha, \beta = 1}^{n} M_{\alpha \beta} \sigma_\alpha \cdot \sigma_\beta . \quad (8)$$

Note that both Hamiltonians have the same interaction topology $M_{\alpha \beta}$, i.e., bit structure. In the continuum limit, the ground state manifold of \ref{eq:4} becomes $SO(3)$-degenerate and contains the separable state $|s\rangle = |\to \cdots \to\rangle$. This degeneracy grants us the freedom of choosing the most appropriate initial state for the adiabatic algorithm. The total angular momentum $\Sigma_z$ around the $z$-axis is conserved during the evolution. In the final state, $\Sigma_z$ counts the difference $\Delta$ between the numbers of zeros and ones in the solution (Hamming weight). Therefore, in order to gain a significant final fidelity, the initial state should be completely contained in the relevant subspace $\Sigma_z \langle \Psi \rangle = \Delta |\Psi\rangle$. A suitable initial state can be generated by the projector

$$|\text{in}\rangle = \frac{1}{2n + 1} \sum_{k = 0}^{2n} \exp \left\{ 2\pi i \frac{\Delta - \Sigma^z}{2n + 1} k \right\} |s\rangle , \quad (9)$$

which is just the Fourier decomposition of the Kronecker symbol $\delta(\Delta - \Sigma_z)$ and involves single-qubit rotations only. Alternatively, one could use an appropriate energy penalty such as $(\Sigma^z - \Delta)^2$, see also \ref{fig:14}. Of course, for this initial state preparation, we have to know $\Delta$. However, this is not a major obstacle: we have found that for the hard instances we consider (see results), the number of ones in the solution is sharply peaked around $\Delta = n/3$. In any case, the overhead of trying every possible value of $\Delta$ scales linear (i.e., polynomial) in $n$.

Numerically, we found that an initial Hamiltonian corresponding to the transversal $x, y$-ferromagnet

$$H_{\text{in}} = -\frac{1}{4} \sum_{\alpha, \beta = 1}^{n} M_{\alpha \beta} \left( \sigma^x_\alpha \sigma^x_\beta + \sigma^y_\alpha \sigma^y_\beta \right) , \quad (10)$$

yields an even better performance than the one in Eq. \ref{eq:4}. In this case, the exact $SO(3)$-degeneracy of the ground state of Eq. \ref{eq:4} is replaced by an approximate $O(2)$-degeneracy (mean-field approximation) generated by $\Sigma_z$, i.e., the state in Eq. \ref{eq:4} has a large overlap with the exact ground state of Eq. \ref{eq:3} in the relevant $\Sigma_z$-subspace.

In order to test the performance of the linear interpolation between the Hamiltonians \ref{eq:3} and \ref{eq:4} proposed here and to compare it with the conventional interpolation scheme used in \ref{fig:3}, for example, we have simulated the adiabatic quantum algorithms numerically \ref{fig:15}. For different qubit numbers $n$, we have randomly generated instances of the exact cover-3 problem with a unique solution in complete analogy to the procedure described in \ref{fig:3}. In addition – as motivated by the comments after Eq. \ref{eq:3} and Ref. \ref{fig:3} – we have also generated hard subsets of uniquely satisfying agreements with especially few clauses. Technically, this was done by keeping those instances that had $m \leq \text{round}(2n/3)$ clauses only.

The results of our numerical simulations are presented in Fig. \ref{fig:4}. For the conventional interpolation scheme \ref{fig:3} applied to randomly generated instances admitting unique solutions, we reproduce the results known from the literature: Fits to the median runtime yield the same quadratic scaling as in \ref{fig:3} and for the corresponding minimum fundamental gap we obtain similar results.
as in [10] (not shown, [11]). However, it becomes visible that for the instances with few clauses (which we believe to be very hard), the performance of the conventional scheme \( \mathcal{R} \) deteriorates significantly. This is consistent with the observation that the minimum gap is considerably smaller for those hard instances than for the other instances with more clauses in the conventional interpolation scheme (data not shown [11]).

In comparison, the novel adiabatic quantum algorithm \((x, y)\)-network based on a linear interpolation between [10] and [11] proposed here yields a superior performance and scaling behavior up to the range of \( n = 20 \) qubits – which becomes even more pronounced for the hard instances. Note that the data points for those hard instances cluster around qubit numbers that can be divided by three, which is probably a consequence of our restriction \( m \leq \text{round}(2n/3) \). Unfortunately, the error bars and the small problem sizes (albeit at the limit of our computational abilities) do not allow to draw conclusions whether the limiting scaling is exponentially or polynomially for this NP-complete problem. However, our results strongly indicate that the scaling is better than that of the Grover search routine with \( T = O(\sqrt{N}) \). Although these results are encouraging, it should be stressed that the average behavior (median) can be quite different from the worst case scenario. Indeed we did also encounter instances for which the required runtime was significantly longer and the associated gap was very small (the median is insensitive to these). In many of these extremal cases, our novel algorithm was still superior, but sometimes the conventional scheme \( \mathcal{R} \) performed better on these instances.

In summary, the analogy to quantum phase transitions facilitates a better understanding of adiabatic quantum algorithms. Apart from the vanishing energy gap at the critical point (in the continuum limit), another typical signature for the occurrence of a phase transition is the divergence of the entanglement, cf. [16]. The energy barrier occurring in first-order transitions provides an intuitive explanation for the exponential scaling of the runtime observed in these situations. The absence of this barrier in transitions of second (or higher) order gives raise to the hope that suitably designed adiabatic quantum algorithms might yield a much better scaling behavior – possibly even an exponential speed-up.

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