Adiabatic quantum computation and quantum phase transitions

José Ignacio Latorre¹ and Román Orús¹

¹Dept. d’Estructura i Constituents de la Matèria, Univ. Barcelona, 08028, Barcelona, Spain.
(Dated: 31st October 2018)

We analyze the ground state entanglement in a quantum adiabatic evolution algorithm designed to solve the NP-complete Exact Cover problem. The entropy of entanglement seems to obey linear and universal scaling at the point where the energy gap becomes small, suggesting that the system passes near a quantum phase transition. Such a large scaling of entanglement suggests that the effective connectivity of the system diverges as the number of qubits goes to infinity and that this algorithm cannot be efficiently simulated by classical means. On the other hand, entanglement in Grover’s algorithm is bounded by a constant.

PACS numbers: 03.67.-a, 03.65.Ud, 03.67.Hk

Quantum adiabatic computation inherently brings the quantum system near to a point where a quantum phase transition takes place. Entanglement is then expected to pervade the system as we shall numerically give evidence when quantum adiabatic computation is applied to the Exact Cover problem, classically classified as NP-complete. Furthermore, scaling of the entropy of entanglement appears to be linear for spin systems with non-local interactions, sub-linear for the XX model, logarithmic for the quantum Ising model and bounded for the Grover’s adiabatic algorithm. In order to substantiate these statements we first need to recall three established results.

Large pure-state entanglement of the quantum register is a key element for exponential speed-up of quantum computation. This result has been made quantitative by Vidal who has proven that a quantum register, such that the maximum Schmidt number of any bipartition is bounded, can be simulated efficiently by classical means. The measure of entanglement proposed in ref. is \( E = \log_2 \chi \), where \( \chi \) is the maximum Schmidt number of any bi-partitioning of the state. It can be further proved that \( E \geq S(\rho) \), where the von-Neumann entropy \( S \) refers to the reduced density matrix of any of the two sub-partitions. If a \( n \)-qubit quantum register only uses little entanglement all along the computation, that is \( \chi = \text{poly}(n) \) at most, both the quantum state as well as the action of the quantum gates on it can be efficiently simulated by classical means. This implies that exponential speed up is only possible if entanglement pervades the quantum register at some point along the computation, that is, if \( \chi \sim \exp(n^a) \), with \( a \) being a positive constant, which is naturally satisfied if the entropy obeys \( S(\rho) \sim n^b \), for some positive constant \( b \). Any algorithm designed to exponentially accelerate a classical computation must create exponentially large \( \chi \). An exponentially big \( \chi \) is therefore a necessary, though not sufficient, condition for quantum exponential speed-up.

On a second separate development, entanglement for the ground state of many quantum spin chain systems has been proven to scale at quantum phase transitions (see also ). The entropy associated to tracing out all but \( L \) spins out of an infinite spin chain displays logarithmic scaling controlled by the central charges, \( c \) and \( \bar{c} \), classifying the universality class of the phase transition \( S_L = \frac{c + \bar{c}}{6} \log_2 L \).

Results from field theory suggest that \( d \)-dimensional spin systems should display a leading scaling behavior completely determined by the area of the region separating the partitioning of the system. For instance, when separating the system in the interior and exterior of a sphere of radius \( R \) and assuming an ultraviolet cutoff \( x_0 \), the entropy of e.g. the interior is

\[
S = c_1 \left( \frac{R}{x_0} \right)^{d-1}
\]

(2)

where \( c_1 \) corresponds to a known heat-kernel coefficient \( \text{R} \). This leading scaling behavior can be cast in terms of the number of spins in the system as

\[
S \sim \frac{d-1}{n^2}.
\]

(3)

Entanglement only saturates for non-critical quantum systems in one dimension \( \text{R} \).

The third element we need to introduce corresponds to the quantum adiabatic computation framework introduced by Farhi et al. (see also ). The quantum register is initially prepared on the ground state of a known initial Hamiltonian \( H_0 \). The system is then made to evolve adiabatically from this Hamiltonian to a new one \( H_P \) whose ground state codifies the solution to an e.g. NP-complete problem

\[
H(s(t)) = (1 - s(t))H_0 + s(t)H_P.
\]

(4)

Slow evolution from \( s(t = 0) = 0 \) to \( s(t = T) = 1 \) guarantees that the system will not jump from the instantaneous ground state of the system to the first excited
state. Quantum adiabatic computation is efficient provided that the minimum gap along the adiabatic evolution is only polynomially small in the number of qubits.

It follows from the above arguments that quantum adiabatic computation can be viewed as a time evolution in which there is a flow along the parameter space defining the Hamiltonian. At a given point $s_c$, the Hamiltonian approaches a quantum phase transition, characterized by a vanishing energy gap. Exponential speed-up needs large entanglement which is also expected at some quantum phase transitions as discussed previously. A quantum computer programmed to find the solution to a given problem using adiabatic evolution does in fact correspond to a system that passes near a quantum phase transition. A quantum computation is thus equivalent to the simulation of a very specific quantum phase transition. Reversely, simulating a quantum phase transition is known to be in general a hard problem that is in principle efficiently solved by adiabatic evolution if the energy gap does not vanish exponentially with the number of qubits.

We shall give support to the above picture by analyzing the span of entanglement along a quantum adiabatic computation applied to the Exact Cover problem, closely related to the 3-SAT NP-complete problem. We shall indeed see that entanglement seems to span over exponentially many states in the computational basis and therefore the algorithm may be hard to simulate in an efficient way using a classical computer. This is a necessary (thought not sufficient) condition for quantum exponential speed-up which is apparently successfully verified in our case.

The NP-complete Exact Cover problem is a particular case of the 3-SAT problem and is defined as follows: given the $n$ boolean variables $\{x_i\}_{i=1,...,n}$, $x_i = 0, 1 \forall i$, where $i$ is the bit index, we define a clause $C$ involving the three bits $i, j$ and $k$ by the constraint $x_i + x_j + x_k = 1$. There are only three assignments of the set of variables $\{x_i, x_j, x_k\}$ that satisfy this equation, namely, $\{1, 0, 0\}$, $\{0, 1, 0\}$ and $\{0, 0, 1\}$. An instance of Exact Cover is a collection of clauses which involves different groups of three qubits. The problem is to find a string of bits $\{x_1, x_2, \ldots, x_n\}$ which satisfies all the clauses.

The Exact Cover problem can be mapped to finding the ground state of a Hamiltonian \(H_P\) in the following way [2]: given a clause $C$ define the Hamiltonian associated to this clause as

\[
H_C = \frac{1}{8} \left((1 + \sigma_i^z)(1 + \sigma_j^z)(1 + \sigma_k^z) + (1 - \sigma_i^z)(1 - \sigma_j^z)(1 - \sigma_k^z) + (1 + \sigma_i^z)(1 + \sigma_j^z)(1 - \sigma_k^z) + (1 - \sigma_i^z)(1 - \sigma_j^z)(1 + \sigma_k^z)\right)
\]

where $\sigma^z|0\rangle = |0\rangle$, $\sigma^z|1\rangle = -|1\rangle$. The quantum states of the computational basis that are eigenstates of $H_C$ with zero eigenvalue (ground states) are the ones that correspond to the bit string which satisfies $C$, whereas the rest of the computational states are penalized with an energy equal to one. The problem Hamiltonian is constructed as the sum of all the Hamiltonians corresponding to all the clauses in the instance,

\[
H_P = \sum_{C \in \text{instance}} H_C.
\]

The ground state of this Hamiltonian corresponds to the quantum state whose bit string satisfies all the clauses. The original problem stated in terms of boolean logic has been cast into the hard task of finding the ground state of a spin system with non-local two and three body interactions. The couplings depend on the particular chosen instance and, therefore, the spin system has not an a priori well defined dimensionality neither a well defined lattice topology, in contrast with the usual spin models (e.g. the anti-ferromagnetic Heisenberg model in a 2-dimensional square grid). This intrinsic relation between physical systems and difficult computational problems is a well established fact. For example, the ground-state search for some spin Hamiltonians defined on regular two-dimensional planar cubic lattices is proved to be an NP-hard problem [10]. Notice that the systems considered in this paper, namely those arising from the Exact Cover problem, differ a lot from those of [10] as long as the detailed structure of the Hamiltonian is considered. Nevertheless, it is a remarkable fact that the Exact Cover problem can be mapped to a ground-state search of a spin-system, as in [10], which provides some physical intuition.

Adiabatic evolution is carried by the $s$-dependent Hamiltonian $H(s)$ as a linear interpolation between an initial Hamiltonian $H_0$ and $H_P$: $H(s) = (1-s)H_0 + sH_P$, where the initial Hamiltonian $H_0$ can be taken as a magnetic field in the $x$ direction

\[
H_0 = \sum_{i=1}^{n} \frac{d_i}{2}(1 - \sigma_i^x),
\]

where $d_i$ is the number of clauses in which qubit $i$ appears. The ground state of $H_0$ is an equal superposition of all the possible computational states. Observe that $H(s)$ is, apart from a constant factor, a sum of terms involving local magnetic fields in the $x$ and $z$ direction, together with two and three-body interaction coupling terms in the $z$ component.

Our numerical analysis is based on the random generation of 300 instances for Exact Cover with only one possible satisfying assignment for $n = 6$ up to $n = 20$ qubits. We produce the instances by adding clauses at random until there is exactly one satisfying assignment, starting over if we end up with no satisfying assignments. According to [4], these are believed to be difficult instances for the adiabatic algorithm. For every instance, we have constructed its corresponding interpolating Hamiltonian.
and found the ground state for $s = 0$ to $s = 1$ in steps of 0.01. We then consider a bipartition of the system into two blocks of $n/2$ qubits and calculate the entanglement entropy between the two blocks as a function of $s$. We have explicitly checked on some instances that all possible partitions produce entropies of the same order of magnitude (as expected from the non-locality of the interactions) and chosen to work with the first $n/2$ versus the rest.

The results we find for the scaling of entanglement seem to agree with the idea that the system approaches a quantum phase transition along its adiabatic evolution. For each of the randomly generated Hamiltonians we observe a peak in the entanglement entropy around a critical value of the parameter $s_c \approx 0.7$. The average entropy shape over the 300 instances is represented in Fig. 1.

In order to analyze how entanglement scales at the critical value $s_c$, we plot the maximum entropy of entanglement as a function of the number of qubits, both for the worst case and for the average over the 300 instances.

The numerical analysis shown in Fig. 2 apparently agrees with linear scaling and matches the expectation that the Exact Cover problem can be viewed as a spin system with highly non-local three-body couplings, and therefore high effective dimensionality. The points can be fitted by a function of the type $E(n) \sim 0.1 n$. This behavior would correspond to a nearest neighbor-like coupling in $d \sim n$ dimensions, thus diverging as $n$ goes to infinity. We note at this point that the evidence of large entanglement present in the ground-state of the system does not say anything about the efficient performance of the quantum adiabatic algorithm. Despite involving a highly quantum-correlated system, the running time of the algorithm would still be inefficient if the gap were exponentially small. This does not seem to be the case, as we shall see, according to our simulations.

Our numerical analysis is also consistent with the work of Farhi et al. in [9] where the minimum energy gap appears to decrease as $g_{\text{min}} \sim 1/n$, as shown in Fig. 3. It is important to emphasize the difference between finding scaling laws for averages and analyzing the worst case. From the point of view of characterizing a phase transition, averages over Exact Cover instances follow quite well defined laws. The worst case is harder to discuss as no systematic search of it can be done. The worst case results can only be considered as consistent with the polynomial vanishing of the energy gap. It is worth noticing that the worst case, defined as the instance with a smaller minimum gap, brings also the higher entanglement as the system is passing closer to the phase transition. Moreover, the minimum gap takes place at the same place where entanglement peaks. This phenomenon is illustrated in Fig. 4 where $s_c$ appears to converge to the same value when $n \to \infty$ from above for the minimum gap and from below for the maximum entanglement.

The scaling of entanglement entropy as the system passes near a quantum phase transition point is asymmetric, as is seen in Fig. 4. The growth of entanglement is slower in the beginning of the evolution and fits remarkably well a curve of the type $E \sim \log|\log(s_c - s)|$, whereas the falling down of the peak is better parametrized by a power law $E \sim |(s - s_c)|^{-\alpha}$ with $\alpha \sim 2.3$. Both scaling behaviors improve as $n$ becomes larger.

Grover’s algorithm [11] does not produce exponential speed-up. It is then arguable that entanglement, despite being necessary for having some computational speed-up, should not play a relevant role in this case. It is indeed possible to analytically address this question. Let
us cast Grover’s algorithm into the adiabatic evolution of the Hamiltonian
\[ H(s) = (1 - s)(I - |s\rangle\langle s|) + s(I - |x_0\rangle\langle x_0|), \tag{8} \]
where \(|s\rangle = \frac{1}{2^{n/2}} \sum_{x=0}^{2^n-1} |x\rangle\), \(n\) is the number of qubits, and \(|x_0\rangle\) is the marked state \([12, 13]\). Other alternative definitions of the Hamiltonian used in Grover’s adiabatic algorithm (such as Hamiltonians explicitly defined in terms of qubits) do not lead to significantly different conclusions from the ones presented in this work. The computation takes the quantum state from an equal superposition of all the possible computational states directly to the state \(|x_0\rangle\), as long as the evolution remains adiabatic. The time the algorithm takes to succeed depends dramatically on how we choose the parametrization of \(s\) in terms of time. The discussion on entanglement can be reduced to analyze its dependence on \(s\) since the explicit dependence on time and its consequences (see \([12, 13]\) for further information about this topic) are of no relevance.

It is straightforward to check that the Hamiltonian \([8]\) has its minimum gap between the ground and first excited states at \(s = 0.5\), which goes to zero exponentially fast as the number of qubits in the system is increased. Therefore, this Hamiltonian seems to undergo a quantum phase transition in the limit of infinite size as \(s = 0.5\) becomes a non-analytical point (for more on the Grover problem as a quantum phase transition, see \([14]\)). We consequently expect quantum correlations to be maximum for this value of \(s\). We present without proof \([15]\) the result of the exact analytical calculation which shows that, for any equally sized bipartition, the entanglement entropy scales as
\[ E(s = 0.5, n \to \infty) = 1 - \frac{4}{\ln 2} 2^{-n/2}, \tag{9} \]
so the entropy tends to 1 for \(s = 0.5\) as an square root in the exponential of the size of the system, which is the typical factor in Grover’s quantum algorithm. Entanglement is also bounded for all possible bi-partitions and no exponential speed up is present. We must remark that our analysis is based on the study of the quantum state between successive calls to the quantum oracle. Entanglement in the quantum register might become very high during the application of the unitary black box, which will in turn depend on the specific searching problem we wish to solve. This very general situation can not be addressed in detail as it depends on the realization of the black box. As long as we restrict ourselves to the situation between calls of the unitary oracle, we see that entanglement is a bounded quantity (which is not necessarily the case along the particular implementation of the quantum black box).

The main theoretical challenge in quantum computation theory remains quantum algorithm design. It has been observed that majorization theory seems to play an important role in the efficiency of quantum algorithms \([16, 17]\). Nevertheless, a relevant element for quantum computational speedup seems to be entanglement \([18, 19, 20]\), and suggest that entanglement grows exponentially (as measured by \(\chi\), the maximum rank of the reduced density matrices obtained over all possible bi-partitions) at a universal point along the adiabatic quantum evolution for the Exact Cover problem, which limits the possibility of an efficient classical simulation. At this point, the system comes close to a quantum phase transition and entanglement obeys a scaling law that needs further investigation. For instance, it has also been proved that entanglement in Shor’s factoring algorithm diverges exponentially fast in the number of qubits, which makes this algorithm difficult to simulate classically as well \([15]\).
Scaling of entanglement seems to be further related to the effective connectivity of the system. Grover’s problem reduces to a two state problem and entanglement is bounded. The quantum Ising, XX and Heisenberg spin chains show logarithmic scaling. Higher dimensional spin models obey faster scaling laws. The maximum connectivity corresponds to non-local interactions (as those present in the adiabatic evolution algorithm for the 3-SAT problem) and entropy does approach its maximum scaling. Computationally hard problems are thus associated to quantum systems that present phase transitions where entropy comes close to its maximum possible scaling.

Acknowledgments: We are grateful to J. Bergli, A. Childs, M. A. Martin-Delgado, E. Rico and G. Vidal for fruitful discussions. We acknowledge financial support from MCYT FPA2001-3598, GC2001SGR-00065, IST-1999-11053, PB98-0685 and BFM2000-1320-C02-01 and the Benasque Center for Science.

[1] E. Farhi, J. Goldstone, S. Gutmann, M. Sipser, quant-ph/0001106
[2] S. Sachdev, Quantum phase transitions, Cambridge University Press, Cambridge (1999).
[3] G. Vidal, J. I. Latorre, E. Rico, A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003), quant-ph/0211074
[4] J. I. Latorre, E. Rico, G. Vidal, quant-ph/0304098
[5] G. Vidal, quant-ph/0301063
[6] C. G. Callan and F. Wilczek, Phys. Lett.B 333 (1994) 55, hep-th/9401072
[7] T. M. Fiola, J. Preskill, A. Strominger and S. P. Trivedi, Phys. Rev. D 50 (1994) 3987, hep-th/9403137
M. Srednicki, Phys. Rev. Lett. 71 (1993) 666-669, hep-ph/9303048
[8] D. Kabat and M. J. Strassler, Phys. Lett. B329, 46 (1994), hep-th/9401125 D. Kabat, Nucl. Phys. B453, 281 (1995), hep-th/9503016
[9] E. Farhi, J. Goldstone, S. Gutmann, J. Lapan, A. Lundgren, D. Preda, quant-ph/0104129
[10] F. Barahona, J. Phys. A: Math. Gen. 15, 3241-3253 (1982).
[11] L. K. Grover, Proc. 28th Annual ACM Symposium on the Theory of Computing, 212 (1996), quant-ph/9605043
[12] J. Roland, N. J. Cerf, Phys. Rev. A 65, 042308 (2002), quant-ph/0107015
[13] W. van Dam, M. Mosca, U. Vazirani, Proc. 42nd Symposium on Foundations of Computer Science, 279 (2001), quant-ph/0206009
[14] A. M. Childs, J. Goldstone, quant-ph/0306054
[15] R. Orús, J. I. Latorre, quant-ph/0311017
[16] J. I. Latorre, M. A. Martin-Delgado, Phys. Rev. A66, 022305 (2002), quant-ph/0111146
[17] R. Orús, J. I. Latorre, M. A. Martin-Delgado, Quant. Inf. Proc., 4, 283-302 (2003), quant-ph/0206134 and quant-ph/0212094
[18] J. Ahn, T. C. Weinacht, P. H. Bucksbaum, Science 287(5452), 463 (2000).
[19] P. Knight, Science 287(5452), 441, 21 (2000).
[20] R. Jozsa, N. Linden, quant-ph/0201143.