Rodríguez-Laguna, Javier, Santalla, Silvia N. (2014). Physical consequences of P[not equal]NP and the DMRG-annealing conjecture. *Journal of Statistical Mechanics: Theory and Experiment*, 7(P07006), 16 pp.

DOI: https://doi.org/10.1088/1742-5468/2014/07/P07006

Physical consequences of P≠NP and the DMRG-annealing conjecture

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(Dated: April 22, 2014)

Computational complexity theory contains a corpus of theorems and conjectures regarding the time a Turing machine will need to solve certain types of problems as a function of the input size. Nature *need not* be a Turing machine and, thus, these theorems do not apply directly to it. But *classical simulations* of physical processes are programs running on Turing machines and, as such, are subject to them. In this work, computational complexity theory is applied to classical simulations of systems performing an adiabatic quantum computation (AQC), based on an annealed extension of the density matrix renormalization group (DMRG). We conjecture that the computational time required for those classical simulations is controlled solely by the *maximal entanglement* found during the process. Thus, lower bounds on the growth of entanglement with the system size can be provided. In some cases, quantum phase transitions can be predicted to take place in certain inhomogeneous systems. Concretely, physical conclusions are drawn from the assumption that the complexity classes **P** and **NP** differ. As a by-product, an alternative measure of entanglement is proposed which, via Chebyshev's inequality, allows to establish strict bounds on the required computational time.

PACS numbers: 05.30.Rt 03.65.Ud 89.70.Eg 03.67.Mn

I. INTRODUCTION

Global optimization is one of the most important computational problems in science and technology. But beyond its practical relevance, it is also of deep theoretical interest when viewed from the broader perspective of computational complexity theory [1, 2]. Problems are ranged into an intrincate classification by theoretical computer scientists, and an impressive corpus of theorems and conjectures has been built to relate them, such as the Cook-Levin theorem [3, 4] which proves the existence of **NP**-complete problems, or the conjecture that **P**≠**NP**.

All those complexity classes are defined with respect to an abstract computer, the *Turing machine*. Physical devices designed to solve a particular problem need not be subject to that restriction, i.e.: an **NP**-complete problem *might* be solved in polynomial time by a physical device even if **P**≠**NP**. The reason is that *Nature need not be a Turing machine*. Notwithstanding, *simulations* of physical processes on classical computers are bound by the previous hierarchy of classes, since they are (approximately) Turing machines. If **P**≠**NP**, any attempt to solve an **NP**-complete problem in polynomial time with a simulation of a physical process on a classical computer must fail. The reasons for the failure must be deducible from the simulation details, and insight about the underlying physical process might be obtained.

Quantum mechanics provides the most promising physical attempt to outperform classical computation, and among all the quantum computational techniques, we will focus on *adiabatic quantum computation* (AQC), also known as *quantum annealing* [5, 6]. The possibility of using AQC to solve **NP**-complete problems in polynomial time is one of the most exciting problems in quantum computation, but it is not addressed in this work. We will focus on *classical simulations* of AQC built upon *matrix product states* (MPS) [7, 8]. Concretely, we will analyse a technique based on an adiabatic extension of the density matrix renormalization group (DMRG) [9, 10], published as *quantum wavefunction annealing* (QWA) [11]. Along with it, we will put forward and discuss the *DMRG-annealing conjecture*, which states that the efficiency of the QWA simulations of AQC is controlled uniquely by the maximal entanglement found during the process.

Being a classical computational technique, DMRG-based simulations of AQC can never solve **NP**-complete problems in polynomial time, unless **P**=**NP**. Accepting **P**≠**NP** and the adiabatic DMRG-conjecture to hold we can put lower bounds on the behaviour of entanglement during AQC processes. In some cases, it allows us to predict the existence of quantum phase transitions.

Our work, thus, puts under a different light ideas that are known in the area. In recent years a new field is being built, known as *hamiltonian complexity*, which considers the computational complexity of performing classical simulations of quantum systems (see [12] for a recent review). In 2003 Vidal showed that a digital quantum computation involving a fixed amount of entanglement could be efficiently simulated using a matrix product representation [7], thus showing that an exponential speed-up was only possible if the MPS bond dimension grows with the input size. But, assuming that the ground state (GS) of a certain hamiltonian can be described as a MPS of fixed dimension, how hard can it be to find it? In 2006, Eisert showed that this problem can be NP-complete [13].

Indeed both results are not hard to reconcile within the DMRG-annealing conjecture framework, as we will show. In 2009 Hastings proved that AQC with fixed gap in 1D would never achieve an exponential speed-up [14], based on his first rigorous proof of an area law in 1D [15].

This paper is structured as follows. In section II we review the basics of adiabatic quantum computation (AQC) (or quantum annealing) [5, 6]. Section III details the quantum wavefunction annealing technique, an adiabatic extension of DMRG, which is illustrated in section IV. The *DMRG-annealing conjecture* is formulated and discussed in section V. Assuming this conjecture to hold, our main results, which are the physical implications of complexity theory, are exposed in section VI. The paper closes with the conclusions and suggestions for further work.

II. ADIABATIC QUANTUM COMPUTATION

Since the seminal article of R.P. Feynman in 1982 [16], physicists have had an increasing interest in the *simulability* of quantum mechanics, which has grown into the field of *hamiltonian complexity* [12]. The difficulties reside in the exponential growth of the dimension of the Hilbert space. Quantum computation was born with the idea of converting this handicap into an opportunity: perhaps clever exploitation of this exponential growth will allow us to achieve an exponential speed-up of classical algorithms, maybe even to solve **NP**-complete problems in polynomial time [17]. This hope has not yet been either fulfilled or disproved, and we will not address it here.

Among the quantum computational techniques proposed, we will focus on adiabatic quantum computation (AQC) [5], studied also under the name of quantum annealing [6, 18]. AQC was proved in 2004 to be *universal* in the sense that the results of any quantum computation can be simulated in polynomial time with an AQC [19].

An AQC is implemented by a physical device which establishes an adiabatic route between two hamiltonians, H_0 and H_1, such that the ground state (GS) of H_0 is easy to obtain physically, and the GS of H_1 provides the solution to some problem. The GS of a hamiltonian is difficult to achieve experimentally when the system is subject to *ageing*, i.e.: when the low energy spectrum is complex, as it happens for most disordered systems. The adiabatic theorem ensures that, *if the process is slow enough and the gap never vanishes exactly*, the ground state of H_1 will be obtained from that of H_0.

As a relevant example throughout this work let us consider the (classical) spin-glass problem [20]. Given a graph $\mathcal{G}$ of N spins and a set of arbitrary real coupling constants J_{ij} attached to each graph link, we define the (classical) spin-glass energy as

$$E = -\sum_{\langle i,j\rangle} J_{ij}\sigma_i\sigma_j \tag{1}$$

Where the σ_i are values in $\{-1,+1\}$ attached to each site. The (classical) spin-glass problem is to find the values for σ_i which minimize the previous energy.

If the graph is 1D, the problem is trivially in **P**. If it is 2D, a non-trivial construction found by Barahona [21] also renders the problem polynomial. For higher dimensions, or for arbitrary graphs of fixed connectivity ($\geq$3), the problem is **NP**-complete [22]. Even a 3D graph composed of two flat layers yields an **NP**-complete problem[21].

The AQC strategy for the spin-glass problem sets the target Hamiltonian, H_1, to be a quantum counterpart of eq. (1), promoting the $\{-1,+1\}$ values of σ_i to spin-1/2 operators [23]:

$$H_1 = -\sum_{\langle i,j\rangle} J_{ij} S_i^z S_j^z \tag{2}$$

On the other hand, the initial Hamiltonian, H_0, must be chosen in such way that its GS is easy to obtain and corresponds to a system subject to very strong quantum fluctuations. A suitable example is the coupling to a uniform transverse magnetic field: $H_0 = -\sum_i S_i^x$. The system will interpolate adiabatically between both Hamiltonians. At all times, it will be described by the Ising model in a transverse field (ITF) with arbitrary couplings:

$$H(\lambda) = (1-\lambda)H_0 + \lambda H_1 \tag{3}$$

$$= -\lambda \sum_{\langle i,j\rangle} J_{ij} S_i^z S_j^z - (1-\lambda)\sum_i S_i^x \tag{4}$$

where we see that $H(0) = H_0$ and $H(1) = H_1$, and λ will be termed the *adiabatic parameter*.

Let $|\Psi(\lambda)\rangle$ denote the ground state of the previous system as a function of λ, which is only degenerate for $\lambda = 1$. If $\lambda = 0$, the ground state is found just by making all spins point in the X-direction:

$$|\Psi(0)\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle + |-\rangle\right)^{\otimes n} \tag{5}$$

In this state, all classical configurations take exactly the same probability, so we may say that it is absolutely disordered. For $\lambda \to 1^-$, on the other hand, the ground state provides the solution to the classical spin-glass problem. Thus, the AQC strategy is to take $\lambda = 0$, increase it adiabatically until $\lambda = 1$ and then read the solution. The adiabatic theorem can be applied if the process is slow enough, assuming that the gap never vanishes exactly.

Of course, in the laboratory it is more convenient to leave the coefficient of H_1 untouched through the procedure. The AQC strategy is to apply a large transverse field initially, and decrease it slowly enough [23]. The main difficulty during an AQC experiment is to ensure adiabaticity. The probability of a jump to an excited

state increases exponentially as the energy gap closes, as reflected by the Landau-Zener formula [23]. Thus, if the system undergoes a quantum phase transition and the energy gap vanishes, the velocity must be reduced in an appropriate way at that point, increasing the computational time.

It may be tempting to try to extract conjectures about the minimal gap along an AQC trajectory from the (classical) complexity class of the problem at hand. But these inferences are *not valid*, since the precise nature of the relation between the quantum and the classical complexity classes is not straightforward. Recent results of Altshuler and coworkers [24] cast doubts on the possibility of solving **NP**-complete problems in polynomial time using quantum computation, due to the very narrow gap distribution in disordered systems which can be expected from Anderson's theorem. Nonetheless, other authors are more optimistic, believing that a route which avoids exponentially small gaps is feasible [25]. Those problems, which are of uttermost importance for quantum computation, will not be studied in this work.

A caveat is in order: AQC is not designed for cases in which the gap is exactly zero at some point. This imposes certain restrictions on H_0 and H_1. For example: an adiabatic calculation in which the Hamiltonian interpolates linearly between the (classical) ferromagnetic Ising model in S^z and a (classical) spin-glass, also in S^z, is not possible. Both Hamiltonians commute, the ground state becomes degenerate at least once, and the adiabatic theorem does not apply.

III. CLASSICAL SIMULATION OF AQC: QUANTUM WAVEFUNCTION ANNEALING

In order to apply the results of computational complexity theory, we should analyse algorithms running on Turing machines, not on arbitrary physical devices. Therefore, we will study *simulations* of adiabatic quantum computation running on a classical computer.

A first simulation approach to AQC is the use of path integral Monte-Carlo methods (PIMC) [23]. This technique does not suffer from Landau-Zener (avoided) level crossings, and the closing of the energy gap does not constitute a problem. Nonetheless, if an attempt is made to solve an **NP**-complete problem using it, it is always found that, at some moment, the system undergoes *critical slowing down*. This forces long relaxation times and reduces the efficiency of the procedure. The exact amount of this reduction is not easy to quantify, due to the different complexity classes associated with probabilistic computation [26].

A different simulation procedure, quantum wavefunction annealing (QWA), is a fully deterministic classical algorithm and lends itself more easily to analysis [11]. The key feature of QWA simulation is that it computes the full wavefunction of the involved ground states. Let $H(\lambda) = (1-\lambda)H_0 + \lambda H_1$, with $\lambda \in [0,1]$. Then, the QWA procedure is:

1. Let $\lambda = 0$ and find the GS of the initial hamiltonian $H(0) = H_0$, $|\Psi(0)\rangle$. Choose a suitable initial value for $\delta\lambda$.
2. Increase the adiabatic parameter: $\lambda' = \min(\lambda + \delta\lambda, 1)$.
3. Find the GS of $H(\lambda')$, $|\Psi(\lambda')\rangle$, *using the previous ground state as a seed*.
4. If the overlap $|\langle\Psi(\lambda')|\Psi(\lambda)\rangle|$ is below a given threshold, halve $\delta\lambda$ and return to 2.
5. If $\lambda' < 1$, make $\lambda = \lambda'$ and return to 2.

If this computation were done in a naive way, the number of stored components would be 2^N, thus rendering it unfeasible. Instead, the wavefunctions may be stored as matrix product states (MPS):

$$|\Psi\rangle = \sum_{s_1 \cdots s_N} \mathrm{Tr}(A_1^{s_1} \cdots A_N^{s_N}) \, |s_1, \cdots, s_N\rangle \qquad (6)$$

where the $A_i^{s_i}$ are $2N$ matrices of size $m \times m$, and m is called the *bond dimension*. The total number of components in a MPS is, therefore, $2Nm^2$. Of course, m must be chosen *so that the ground state is always accurately represented*. The required value of the bond dimension m will be, therefore, of uttermost importance in order to evaluate the efficiency of the procedure.

Our technique of choice in order to determine the MPS representation of the ground state for each value of Γ is the density matrix renormalization group (DMRG) [9, 10]. The technique has several important features:

- DMRG is variational within the MPS subspace of the Hilbert space.
- DMRG allows for adaptable values of m. In QWA simulations, m must be an *adaptable* parameter, which is chosen to be large enough to represent the state accurately at each simulation stage, to a given tolerance.
- DMRG benefits from the use of a *seed state* in order to accelerate convergence, via the so-called *wavefunction transformations* [27].

Thus, the QWA algorithm under consideration is just an annealed extension of the DMRG.

There are other algorithms to simulate a quantum computation based on the MPS representation, e.g. the algorithm by Vidal [7] for digital quantum computation or the one by Bañuls and coworkers [28] for AQC. The latter case uses real time simulation, which may lead to a new source of loss of adiabaticity. Nonetheless, they both point to similar relations between entanglement and the efficiency of the calculation.

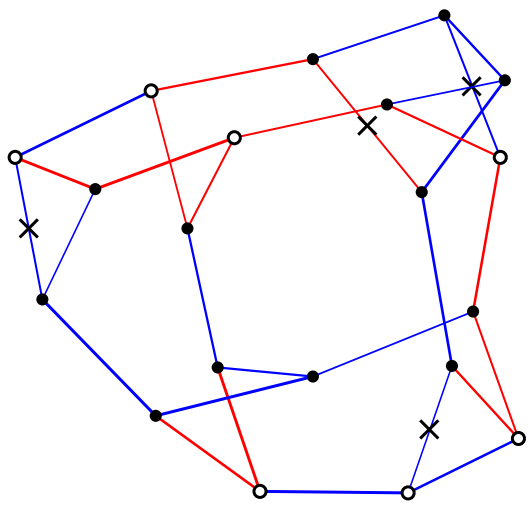

FIG. 1. Illustration of a spin-glass problem instance solved by QWA. Red links are *antiferromagnetic*, and blue ones are *ferromagnetic*, with their width increasing with their strength. Sites are represented by either empty or full circles, denoting that the solution is either + or −. The frustrated links in the optimal solution are marked by a cross.

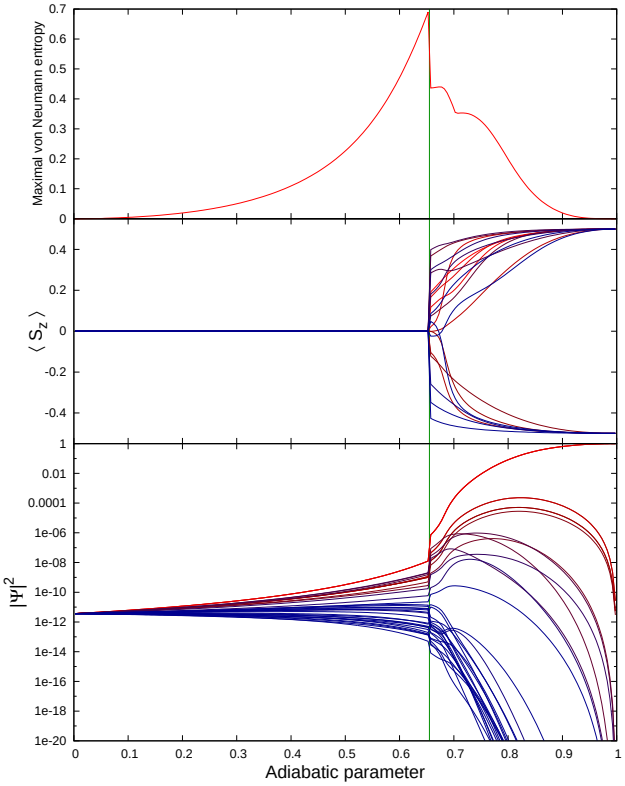

FIG. 2. Development of the QWA algorithm. Top: evolution of the maximal von Neumann entanglement found at different stages of the simulation. Notice the peak at $\lambda_c \approx 0.655$, denoting the quantum spin-glass phase transition. Center: Magnetization of each spin; notice the strong jump exactly at λ_c, and how not all the spins grow at the same rate. Bottom: Weights of different selected configurations, eq. (7), color denotes classical energy (red is lowest). They all start at $1/2^N$, and spread uniformly up to λ_c, when the transition takes place. Only the actual optimum reaches 1, all the rest fall eventually to zero.

IV. ILLUSTRATING THE QUANTUM WAVEFUNCTION ANNEALING

The efficiency of QWA was analysed in [11] on the random ITF model given by eq. (4) for quasi-2D systems and random graphs of fixed connectivity, and the results in that article give support to the idea that the method will always reach the classical minimal energy, provided that it is allowed to retain as many states as desired. As a means of illustration, fig. (1) shows a sample graph with $N = 20$ sites and connectivity $K = 3$, along with the QWA solution of the associated classical problem. Links are colored either red (antiferromagnetic) or blue (ferromagnetic), with a width proportional to its strength. Sites are depicted by either filled or empty circles, representing + and − values of the spin. The links marked by a cross are frustrated.

A technical point is in order: the final values of the spins are obtained by measuring S_z on each site. Of course, for the exact GS of Hamiltonian (4), those values will be zero. A negligible longitudinal field in the Z-axis is introduced in order to break the symmetry between the two identical solutions.

Fig. (2) we illustrate how the QWA procedure develops. The horizontal axis is common for all three plots, and represents the advance of the adiabatic parameter λ. On the top panel, we show the evolution of the maximal von Neumann entropy found in the procedure. Notice the peak it presents at $\lambda_c \approx 0.655$, which marks the quantum spin-glass phase transition. There are secondary maxima, which are typical in those cases [29]. The central panel shows the evolution of the expectation values of S_z on each spin during the QWA. For $\lambda < \lambda_c$, i.e.: in the paramagnetic phase, the values are very close to zero. At λ_c, they start a very fast increase, whose rate is not uniform among them. For $\lambda = 1$, they all take values $+1/2$ or $-1/2$, and their signs will provide the solution of the classical problem.

It is possible to define a *weight* for each classical spin configuration $C = \{s_1 \cdots s_N\}$:

$$|\Psi_C|^2 \equiv |\langle s_1 \cdots s_N | \Psi \rangle|^2 \tag{7}$$

i.e.: the probability for each configuration. Within the DMRG, it is possible to obtain accurate estimates for the weights of different configurations, just making use of the MPS structure [11]. We have traced the weights for the actual optimal configuration and a several others, and plotted them as a function of λ in the bottom panel

of fig. (2). The color of the line is an indicator of its energy as a classical configuration, with red being the lowest energy and blue the highest. Notice that, up to λ_c, all weights spread uniformly. At λ_c, the quantum spin-glass phase transition takes place, and a few low-energy configurations start to increase their weight, while most of them decrease very fast. That increase, nonetheless, is only sustained by the classical optimum, which reaches one, while all others fall to zero eventually before $\lambda \to 1$.

V. THE DMRG-ANNEALING CONJECTURE

Let $M(N)$ represent the maximal bond dimension achieved during a certain QWA procedure as a function of the system size. Let us now state the *DMRG-annealing conjecture*:

1. The QWA algorithm, as described above, always obtains the true optimum.

2. The QWA-time is $O(N \cdot M(N)^k)$, for a certain k.

In other words, QWA simulations will always obtain the true optimum of the problem in a time that depends polynomially on the maximal bond dimension. Thus, the QWA procedure will work in polynomial time in the system size whenever the bond dimension grows at most polynomially with N. Also, if the maximal bond dimension $M(N)$ does not grow with N, the QWA time will scale linearly with the system size. In this section we will discuss the arguments in favour of this conjecture, and its possible pitfalls.

A first argument supporting the conjecture is the result by Vidal [7] stating that a digital quantum computation which involves a finite amount of entanglement can be efficiently simulated using a classical computer. One should realize, nonetheless, that this result, as such, is not applicable to the case of adiabatic quantum computation. Indeed, digital and adiabatic quantum computation have the same power [19], but their classical simulations need not be equally amenable. The results of [7] have not been extended to generic AQC on an arbitrary graph, but only to dynamical simulations in 1D [30].

Of course, the MPS representation of the wavefunction is highly dependent on the *ordering* of the sites in the system, since the maximal bond dimension, $M(N)$, can be strongly dependent on it. As an example, the bond dimension for a non-critical 1D system saturates if the natural ordering is chosen, but if our ordering is $\{1, 3, 5, 7, \cdots, 2, 4, 6 \cdots\}$, the bond dimension will grow exponentially with the system size [31]. In QWA, the ordering manifests in the choice of the *DMRG-path*. In absence of a natural 1D structure, finding the path that minimizes the bond dimension is a hard problem. It can be tackled approximately taking profit of the *area law*, i.e.: assuming that entanglement (and, thus, the bond dimension) of a division of the system will increase with the number of broken bonds. Low-cost heuristical approaches to this problem are discussed in [11, 29].

Let us consider the eigenvalues of the reduced density matrix ρ found at any stage of the DMRG procedure. They constitute a discrete probability distribution, $\{p_i\}_{i=1}^{N_T}$, which we will assume to be in decreasing order. Assuming a certain bond dimension m is equivalent to the approximation of retaining the first m eigenvalues p_i and neglecting the rest. Given a certain tolerance $\epsilon > 0$, we would like to find $m(\epsilon)$, the minimum number of eigenvalues that must be retained so that the sum of the remaining ones is smaller than ϵ:

$$\sum_{i>m(\epsilon)} p_i < \epsilon \tag{8}$$

The von Neumann entropy of entanglement is the Shannon entropy of the eigenvalues of ρ: $S \equiv \langle -\log(p_i) \rangle$. In the DMRG literature it is usually assumed that the required bond dimension $m(\epsilon)$ scales as the exponential of the von Neumann entropy of entanglement [10], $m(\epsilon) \approx \exp(S)$. It is straightforward to show that, given a MPS of dimension m, the maximal von Neumann entanglement that it can sustain is, indeed, $\log(m)$. Thus, $m(\epsilon) > \exp(S)$. But this scaling $m(\epsilon) \approx \exp(S)$ can only be proved rigorously for some mild distributions of the eigenvalues of the density matrices. If the eigenvalues decay exponentially, it can be proved that for all $\epsilon > 0$, $m(\epsilon) \propto \epsilon^{-1} \exp(S)$. In case of slower decays, still a polynomial relation can be found between $\exp(S)$ and $m(\epsilon)$, but this is not true for generic distributions.

Instead of the von Neumann entropy, we can employ a different measure of entanglement, such as the average and variance of the *eigenvalue index*:

$$\mu_i \equiv \sum_{i=1}^{N_T} i \cdot p_i \tag{9}$$

$$\sigma_i^2 \equiv \sum_{i=1}^{N_T} i^2 \cdot p_i - \mu_i^2 \equiv \left\langle i^2 \right\rangle - \left\langle i \right\rangle^2 \tag{10}$$

With this new measure of entanglement, Chebyshev's inequality directly provides the possibility of a rigorous relation:

$$m(\epsilon) = \mu_i + \frac{1}{\sqrt{\epsilon}} \sigma_i \quad \Rightarrow \quad \sum_{i>m(\epsilon)} p_i < \epsilon \tag{11}$$

Therefore, whenever μ_i and σ_i are finite for every partition during the DMRG process, we have a rigorous bound on the bond dimension required for any given tolerance. Figure (3) shows the behavior of these measurements of entanglement along the QWA process which served as illustration in section (IV). For this figure, we have obtained the maximal value of μ_i and of σ_i, independently, as a function of the adiabatic parameter.

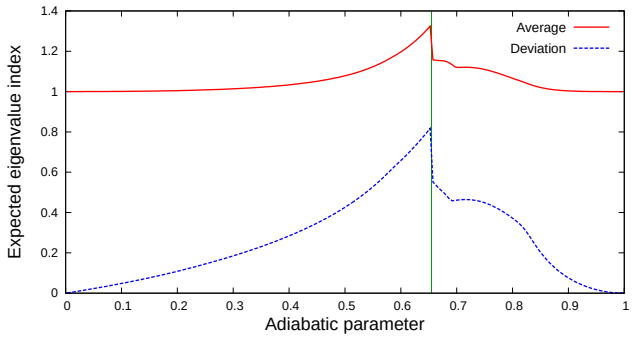

FIG. 3. Maximal average and maximal deviation of the eigenvalue index of the reduced density matrix during the QWA procedure described in sec. IV.

Once that a technique has been provided to find the required bond dimension $m(\epsilon)$ as a function of the DMRG tolerance, there is a still a question to be addressed: *should the tolerance ϵ depend on the system size for the QWA algorithm to succeed with certainty?* The DMRG-annealing conjecture claims that this is not the case [11]. The validity of this claim rests only in limited empirical evidence, and requires further investigation.

Another claim involved in the DMRG-conjecture is related to the speed at which we are allowed to change λ. At each QWA step, the algorithm attempts to transform the GS at a value λ into the GS at a slightly larger value, $\lambda+\delta\lambda$, by carrying out as many DMRG sweeps as necessary. The cost of each DMRG sweep scales polynomially in m. Thus, we need that the *number* of DMRG sweeps does not scale appreciably with the system size, i.e.: the states $|\Psi(\lambda)\rangle$ and $|\Psi(\lambda+\delta\lambda)\rangle$ must be so close that the transformation can be done in $O(1)$ DMRG sweeps. This can always be achieved by reducing drastically $\delta\lambda$, but this might increase drastically the computational time. The claim is, therefore, that the *total* number of sweeps required for the QWA computation, summing for all the values of λ, does not scale appreciably with the system size. The community consensus is that the DMRG is surprisingly robust in this respect [32], but no proof or counter-example of this claim is known to us.

The QWA algorithm might be improved by taking an *adaptive* value of $\delta\lambda$, estimated at each step from the fidelity, $|\langle\Psi(\lambda)|\Psi(\lambda+\delta\lambda)\rangle|$ [33]. Finding a relation between these two values ensuring a constant number of DMRG-sweeps would provide a valuable insight into the previous claim, and also the means to accelerate the procedure.

Some recent works have been devoted to study the efficiency of the computation of MPS. Finding the ground state of a 1D quantum Hamiltonian can be even **NP**-complete [13, 32]. If m is fixed, instead of adaptable, MPS are always nicely approximable [34]. This means that it is always possible to obtain the best fixed-m approximation to the GS of a given Hamiltonian, within a factor $(1+\epsilon)$ of the ground state energy, polynomially both in time and in ϵ^{-1}. The complexity class which conveys this is called *fully polynomial-time approximation scheme* (**FPTAS**) [35].

Since the efficiency of the procedure is controlled by entanglement, via the maximal-MPS dimension, let us summarize the known results regarding its behaviour. Gapped systems usually fulfill the *area law* [36, 37], which states that the von Neumann entanglement entropy S between two parts of a system scales as the number of broken links among them. This result was proved rigorously in gapped 1D systems by Hastings [15]. In some higher dimensional inhomogeneous and/or disordered systems it is known not to hold [38, 39]. Moving to critical points, the von Neumann entropy S has proved to be a very useful magnitude in order to pinpoint quantum phase transitions (QPT) [29]. During any adiabatic process with finite N, S always presents a local maximum at a QPT. It has also been conjectured that a non-analyticity of S may constitute a good indicator of a QPT [40]. The 1D case is again rather special: at criticality, S will scale with the system size. In some cases, the size-dependence of S can be found via conformal field theory (CFT) [41]. It has been shown that, for many critical 1D problems, $S(N) \approx \alpha\log(N)+\beta$. Thus, assuming that the bond dimension $m \approx \exp(S)$, it will grow polynomially with the input size.

VI. PHYSICAL IMPLICATIONS OF COMPLEXITY THEORY

A. General principles

Throughout this section, we will adopt the notation that a family of Hamiltonians belongs to a complexity class if the problem of finding the ground state of a generic instance in that family belongs to that complexity class. Unless otherwise stated, we will assume the DMRG-annealing conjecture to hold.

A complexity class which is simpler than **P** is **LIN**, i.e.: the class of problems that can be solved in *linear* time. Let us consider a *fixed* adiabatic route connecting Hamiltonians H_0 and H_1, such that H_0 belongs to a family in **LIN** but H_1 belongs to a family of higher complexity. E.g., H_1 is taken from **P**, but with computational time scaling faster than N, perhaps only $N\log(N)$. Then the bond dimension must *diverge* at some point during the adiabatic route. Typically, this implies that the von Neumann entropy will also diverge. This divergence is typically the hallmark of a quantum phase transition (QPT).

The reason can be stated as follows. Let us assume that the entanglement stays bounded during the whole AQC procedure. Now, let us use a classical computer to run a QWA simulation of the AQC procedure, in time $T(N)$. If the maximal bond dimension saturates with N, QWA results asymptotically in a linear algorithm to obtain the ground state of H_1, against the assumption. Therefore, entanglement must grow without bound with the system size at some moment during the AQC proce-

dure, pointing to a QPT.

In the same line, if H_0 is **P** and H_1 is **NP**-complete, and **P**≠**NP**, then any AQC connecting the two Hamiltonians will find, at some moment, a state with maximal bond dimension growing faster than polynomially in N. Typically this implies that the von Neumann entropy will grow faster than logarithmically with N. This state may correspond to a QPT. Again the reason is easy to state: otherwise, the classical simulation will provide a polynomial algorithm to solve an **NP**-complete problem.

In general terms, we may say that the adiabatic connection of two Hamiltonians within different complexity classes puts restrictions on the physics along the path. In order to avoid violations of the results from complexity theory, entanglement must diverge at some moment during an AQC procedure. This divergence may take place as a quantum phase transition of a certain kind. It can be regarded as a kind of *quantum censorship* to prevent hard problems from being solved easily.

Of course, the adiabatic route connecting H_0 and H_1 must be *fixed*, i.e.: established beforehand for all elements of the family. If we allow it to be problem-dependent, there is always a trivial way to find an adiabatic route with no entanglement which requires to know the solution of the classical problem. E.g.: in order to solve the spin-glass problem: (1) get the ground state of $H_0 = -\sum_i S_i^x$, (2) rotate each spin independently and adiabatically until they reach their solution value σ_i, by shifting to $H_{1/2} = -\sum_i \sigma_i S_i^z$ and (3) change adiabatically to $H_1 = -\sum_{\langle i,j\rangle} J_{ij} S_i^z S_j^z$.

In this framework, it is easy to reconcile the apparently contradictory results cited in the introduction. Vidal proved that a digital quantum computation involving a finite amount of entanglement can be efficiently simulated [7], and Eisert proved that the obtention of the GS of a Hamiltonian can be **NP**-complete *even* if it is described by a MPS of low bond dimension [13]. The DMRG-annealing conjecture predicts that any AQC designed to find such GS, no matter the starting point or the adiabatic route followed, will find a state with unbounded entanglement, most probably a quantum phase transition. Thus, both results are reconciled.

This analysis is independent of whether we focus on average or worst-case complexity. Once the set of problems is characterized, and a bound on the computational time is established, it can be immediately converted into a bound for the entanglement entropy for an AQC.

A relevant point to be made is how to know whether the divergence of the maximal entanglement points to a quantum phase transition or not. In 1D it is known that at a QPT both the entanglement entropy and the bond dimension diverge [15]. In higher dimensional studies, a more careful analysis is required, since the maximal bond dimension is likely to diverge along the whole AQC procedure. In any case, for any finite instance of a problem, the maximum attained by the entanglement determines the efficiency of the QWA. Therefore, if a QPT is present, even if the bond dimension diverges with N at all points during the AQC, it is the scaling of entanglement at the QPT which establishes the running time for the simulation.

B. Concrete examples

Let us return to the spin-glass hamiltonian (4). When $\lambda \to 0$, the obtention of the ground state is a trivial problem, taking $O(1)$ time. In 1D, the obtention of the classical spin-glass minimum energy state is obviously in **LIN**. Therefore, our results do not apply in this case, since QWA takes always time $\geq N$.

In 2D, on the other hand, a prediction can be done. Solving the 2D classical spin-glass problem is known to be in **P**, but not in **LIN** [21]. Therefore, entanglement must diverge for some value of λ. We can only state that the maximal entropy will grow, *at least*, logarithmically. In fact, recent results [39] (cleverly exploiting the properties of the infinite randomness fixed point [42], IRFP) show that it grows with a modified area law: for a block division cutting l links, the entropy scales as $s(l) \approx l\log(\log(l))$. Maximal entropy, as it is defined in this work, would be $S(N) \approx N^{1/2}\log(\log(N))$, thus rendering the time for the QWA simulation exponential. Our result is, therefore, valid but too weak.

Nonetheless, the previous expression for the block entropy in a 2D quantum spin-glass is based on the average number of clusters cut by the block division. A well designed DMRG path might never cut more than one cluster at a time, just sweeping them one by one. In that case, the maximal entropy might grow much more slowly with the system size. But, in order to obtain such a path, one should *first* solve the classical problem. Therefore, again, our basic result is not violated.

In 3D, or for random graphs of fixed connectivity, the **NP**-completeness of the problem forces the maximal entropy along the route to grow faster than $\log(N)$. In this case, the result is not surprising.

Other analysis have been carried out for the entanglement entropy along typical standard quantum computations, and our general statements also hold [43]. An AQC designed to solve the *exact cover* problem (which is **NP**-complete) found a QPT with $S \approx N$ [43]. Although not an AQC, Shor's algorithm also shows a similar behaviour. In this case, though, it is not clear which is the complexity class of the problem under study (i.e.: *integer factorization*) [43].

A different type of behavior is found in the *unsorted search* problem, where the input is a set of N values, among which we must find a given one. This problem is in **LIN** so, in consequence, an AQC designed to solve using N qubits may work with bounded entanglement. Nonetheless, the standard adiabatic implementation of Grover's algorithm [44] works using only $n = \log_2(N)$ qubits, yet the maximal entanglement among them is also found to be bounded [43]. This is apparently in contradiction with our prediction, since DMRG would take

a time polynomial in n, which is always smaller than N, which is the classical computation time. The explanation of this apparent paradox is that the approach in [44] makes use of an *oracle function*, which is a non-local external element to the QWA formalism and can not be used in the DMRG.

New predictions are easily made for AQC designed to solve problems which have never been studied. Thus, an AQC designed to test planarity of a graph, or 2-colorability, need not find a quantum phase transition, since these problems belong to class **LIN**. But an AQC which sorts a set of numbers, or which performs the fast Fourier transform, will find a divergence in the bond dimension and, very likely, in the von Neumann entropy, since their running time is larger than linear. The maximal entropy in those cases might grow very slowly with size, since the (average) running time for the best algorithms are $T \approx N \log(N)$, so our only bound is that S should scale at least like $\log(\log(N))$. On the other hand, if **P**≠**NP**, any AQC attempt to solve the traveling salesman problem, or 3-SAT, will always find maximal entropy growing faster than logarithmically.

VII. CONCLUSIONS

Theoretical physics has benefitted continuously from the incorporation of the results of pure mathematics which were born without any relation to it. Computational complexity theory is just another branch of mathematics, and this work just attempts to extract its most straightforward consequences for physics. As Nikolai Lobachevski put it: *"There is no branch of mathematics, however abstract, which may not someday be applied to the phenomena of the real world"* [45].

In this work we have put forward a strategy to derive physical inferences from computational complexity theory. If a physical process is devised in order to solve some problem, simulating that process in a (classical) computer constitutes a (classical) algorithm to obtain the solution. The efficiency of this algorithm may be restricted by complexity theory, and this restriction must have some counterpart in the physical model which may apply to the real physical system.

Concretely, adiabatic quantum computation (AQC) may be simulated in classical computers using quantum wavefunction annealing (QWA), which is a simulation strategy based on the density matrix renormalization group (DMRG). The efficiency of QWA is conjectured to be controlled by the maximal entanglement attained during the physical process. Different measures of entanglement are discussed (bond dimension and von Neumann entropy) and a new one is introduced (variance of the eigenvalue index). Arguments are given in favour of this conjecture, along with an exposition of its possible pitfalls.

If there is a bound on the scaling of the computational time to solve the problem on a classical computer, then this bound will transform itself into another bound for the maximal entanglement attained during the real physical procedure. This type of no-go reasoning bears resemblance to the second law of thermodyamics. In this way, the divergence of entanglement with the system size for some systems is proved. This divergence, in some cases, may be viewed as the apparition of a quantum phase transition, which can be regarded as a "quantum censor", preventing the solution of hard problems in an easy way (in a classical computer).

The main possible pitfalls for the DMRG-annealing conjecture are the following. It is not currently known what tolerance can be accepted in the sum of neglected weights in DMRG in order to ensure the validity of the QWA algorithm. The DMRG-annealing conjecture assumes that this tolerance does not depend on the system size. Also, the total number of DMRG sweeps needed to transform the wavefunction along the adiabatic route is assumed to be independent of the system size. There is limited empirical evidence supporting those claims. Our future work will be devoted to the evaluation of the validity of these assumptions.

The present derivation was performed using matrix product states (MPS) and the DMRG, which are not specially well suited for multidimensional systems, due to the need for a 1D path to run through the system. Different generalizations of MPS exist, such as multiscale entanglement renormalization Ansatz [46] (MERA) or projected entangled pair states [47] (PEPS), which are altogether labeled as tensor networks [48, 49]. New techniques have been developed for 2D optimization problems, making use of ideas related to *dynamic programming* [50, 51]. Also, other techniques have been proposed in order to simulate real time evolution in the Heisenberg picture [52]. We expect that application of this line of thought to these sophisticated tools will provide stronger predictions on the physics found during the performance of an adiabatic quantum computation.

ACKNOWLEDGMENTS

This work has been supported by the Spanish government by grants FIS2012-33642 and FIS2012-38866-C05-1 and ERC grant QUAGATUA. The authors wish to acknowlege very useful discussions with G. Sierra, M. Lewenstein, I. Rodríguez, D. Peralta-Salas and E.H. Kim.

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