Information Theory and Computation Course - Final Project

Adiabatic Quantum Computing for Random Ising Model

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Abstract

The purpose of this paper is of presenting the study of the adiabatic quantum computing for solving a random Ising model Hamiltonian.

1 The adiabatic quantum computing

First of all, it is essential to make a recall about what the adiabatic quantum computing is. From [1]: suppose that we have a quantum Hamiltonian $\hat{H}_T$ whose ground state encodes the solution to a problem of interest, and another Hamiltonian $\hat{H}_0$, whose ground state is "easy" (both to find and to prepare in an experimental setup). Then, if we prepare a quantum system to be in the ground state of $\hat{H}_0$, and then adiabatically change the Hamiltonian for a time T according to

$$\hat{H}(t) = \left(1 - \frac{t}{T}\hat{H}_0\right) + \frac{t}{T}\hat{H}_T \,, \tag{1}$$

then if T is large enough the quantum system will remain in the ground state for all times, by the adiabatic theorem of quantum mechanics. This last theorem is the one that has to quantify the exact nature of that "large" T; the time evolution is instead governed by the usual Schrödinger equation

$$i\frac{\partial \left|\psi(t)\right\rangle}{\partial t} = \hat{H}(t)\left|\psi(t)\right\rangle \tag{2}$$

(we set $\hbar = 1$ from now on).

The adiabatic theorem exists in many variants; for the purpose of this work, it was retained enough to use an approximate version, which however gives rise to a widely used criterion for the time T [2]. Let $\lambda_i(s)$ denote the i-th eigenvalue of $\hat{H}(s)$ at time $s = t/T \in [0, 1]$, such that $\lambda_i(s) \leq \lambda_{i+1}(s) \leq \ldots$, and $|\psi_i(s)\rangle\, (j \in 0, 1, 2, \ldots)$ denotes the respective eigenstate. The adiabatic condition is then the following: [2]

$$\max_{s\in[0,1]} \frac{\left|\langle\psi_i(s)|\, \partial_s \hat{H}(s)\, |\psi_j(s)\rangle\,\right|}{|\lambda_i(s) - \lambda_j(s)|^2} \ll T \quad \forall i \neq j \,. \tag{3}$$

In this work we are interested in evolving the ground state of the system; therefore we can define

$$\epsilon_i = \left|\langle\psi_i(s)|\, \partial_s \hat{H}(s)\, |\psi_0(s)\rangle\,\right| \tag{4}$$

and

$$g_i = |\lambda_i(s) - \lambda_0(s)|^2 \,, \tag{5}$$

and the interesting relation for us will be

$$T \gg \max_{s\in[0,1]} \frac{\epsilon_i(s)}{g_i(s)^2} \,. \tag{6}$$

In this paper the quantity on the right will be often called "estimator".

2 The random field Ising model

The purpose of this work is of using the adiabatic quantum computing to study the ground state of the random field Ising model defined by the Hamiltonian:

$$\hat{H}_T = \sum_{i=1}^{N} \lambda_i \sigma_i^x \sigma_{i+1}^x, \qquad \lambda \in [-1, 1] \tag{7}$$

using as the "easy" Hamiltonian:

$$\hat{H}_0 = \sum_{i=1}^{N} \sigma_i^z \,; \tag{8}$$

the total Hamiltonian for the adiabatic quantum computing is therefore

$$\hat{H}(s) = (1 - s)\hat{H}_0 + s\hat{H}_T \,. \tag{9}$$

At $s = 0$ the system is prepared in the ground state of $\hat{H}_0$, i.e. the one where all the spins are aligned along the opposite direction of the field along the $\hat{z}$ axis; this state is non degenerate with eigenvalue equal to $-N$, the opposite of the number of particles. The next states are found flipping the spins one at a time: the first excited will have an energy equal to $-N + 2$ (with a certain degeneracy), and so on. At $s = 1$ the external field disappears and there is only the interaction Hamiltonian; the sign and the strength of the interaction between two nearest neighbour spins is determined by their coefficient λ: two near spins have a negative interaction if they point in the same direction (along the $\hat{x}$ axis) with $\lambda < 0$, or if they have opposite direction with $\lambda > 0$. Here the ground state has degeneration two, by the moment that flipping all the spins doesn't change the energy. The spectrum strongly depends on the various λ_i: for example, the ground state has energy

$$E_{\text{gs}} = -\sum_i |\lambda_i|$$

and the excited states will have an energy that is also a sum of the lambdas, some ones taken with the + sign and some others with the −; this depends on the particular configuration of these.

Now, it is necessary to spend some words about the parity of the eigenstates of $\hat{H}(s)$, since this will be fundamental in the rest of the of the paper. Let's define the parity operator as follows:

$$\hat{P} = \prod_{i=1}^{N} \sigma_i^z \tag{10}$$

where the product symbol entails a tensor product. For all the cases that will be considered in below, it has been verified that

$$[\hat{H}(s), \hat{P}] = 0 \ : \tag{11}$$

by the moment that s is just an external coefficient (the elements of H_0 and H_T do not depend on s), if that commutator is zero for one value of s, it is zero for any. Also

$$[\hat{H}_T - \hat{H}_0, \hat{P}] = 0 \, , \tag{12}$$

where

$$\hat{H}_T - \hat{H}_0 = \partial_s \hat{H}_s \, . \tag{13}$$

We recall that if a Hamiltonian commutes with the parity operator, then its eigenvectors can be searched through the even and the odd eigenvectors (that are orthogonal), where these are the eigenvectors of the parity operator with eigenvalue respectively +1 and −1. Therefore, applying one of those Hamiltonians on a state with defined parity, won't change the parity of that state. Because of Eq.13, in our case the Eq.4 becomes

$$\epsilon_i = |\langle \psi_i(s)| \, \hat{H}_T - \hat{H}_0 \, |\psi_0(s)\rangle \, | \tag{14}$$

and this is equal to 0 if $|\psi_i\rangle$ has not the same parity of the ground state.

3 A numerical code for simulations

In order to simulate the system described above, the author developed a code in Fortran, which we are going to discuss in its main parts. The code essentially has to:

1. Build the desired Hamiltonian
2. Make the time evolution of the ground state of $\hat{H}_0$
3. Compute the "true" ground state of $\hat{H}(s)$ at each time step for check.
4. Compute the estimator of Eq.6.
5. Calculate commutators, parities, control quantities,...

The following simple subroutine can fulfill the first task:

```
SUBROUTINE TOTAL_MF(ham0, hamp, tt, bigt, total)
    REAL*8 :: tt, bigt
    TYPE(RMATRIX) :: ham0, hamp, total
    total%elem = (1-tt/bigt)*ham0%elem +
                 tt/bigt*hamp%elem
    RETURN
END SUBROUTINE
```

the user can define its Hamiltonians $\hat{H}_0$ and $\hat{H}_T$, and the subroutine computes $\hat{H}(t)$ for each $t \in [0, T]$.
Let's now move to the second point. First of all, $\hat{H}_0$ must be diagonalized in order to obtain the starting ground state, and this is done through the `DSYEV` subroutine provided by Lapack. The most problematic part is now the time evolution, that is performed through the Crank-Nicholson method. The interval $[0, T]$ is discretized in a certain number of steps of size Δt, and the time evolution operator is expanded as follows

$$e^{-i\hat{H}(t)\Delta t} \approx (\mathbb{1} - i\hat{H}\Delta t) + O(\Delta t)^2 \approx \\ \approx \left(\mathbb{1} + \frac{i\hat{H}(t)\Delta t}{2}\right)^{-1} \left(\mathbb{1} - \frac{i\hat{H}(t)\Delta t}{2}\right) + O(\Delta t)^2 \tag{15}$$

The time evolution is performed step by step solving the system of linear equations:

$$\left(\mathbb{1} + \frac{i\hat{H}(s)\Delta t}{2}\right) \psi(t + \Delta t) = \left(\mathbb{1} - \frac{i\hat{H}(s)\Delta t}{2}\right) \psi(t) \, ; \tag{16}$$

this task has been performed through the `ZGESV` subroutine provided by Lapack. At each step the energy relative to the found state was computed simply by doing the expectation value.
The third and the fourth task are achieved both by the same subroutine, that essentially diagonalizes $\hat{H}(t)$ at each step using `DSYEV`, hence providing full knowledge about the eigenstates and the eigenvalues of the Hamiltonian at each step; then it is straightforward to calculate ϵ_i and g_i. Unfortunately, the diagonalization operation soon faces the limits of the computing device: in a computer with 8GB of RAM, a system with more than 15 particles can not even be tackled, and from $10 - 11$ particles on the computation starts to be slow (see Sec.5 for further details).
Concerning the last point, we just mention the control of the parity: the parity operator is built following the definition for a given input dimension, and it is used to calculate the expectation value of the given eigenstate $\psi_i(t)$ of $\hat{H}(t)$. Finally, his same ode was slightly modified in order to be able to take as input given values for the lambdas, in order to study many cases of the random field for a given dimension of the system.

4 A first simple but non trivial system: three particles

Now the results and the analysis for the system made of three particles are discussed; the system with $N = 3$ has been chosen in place of the one with $N = 2$ because it gives at soon the chance of examining the level crossing phenomenon between higher levels.

As first, let's examine the whole spectrum, obtained diagonalizing $\hat{H}(t)$ at each step in the following cases, concerning the two values of λ:

λ_1	λ_2
1	1
0.1	0.1
0.995119	0.133649

In the first two cases we have a uniform field, first strong, and then weak, while in the third case we have the two random values for which a full analysis will be shown in below. Spectra are shown in Figg.1,2,3.

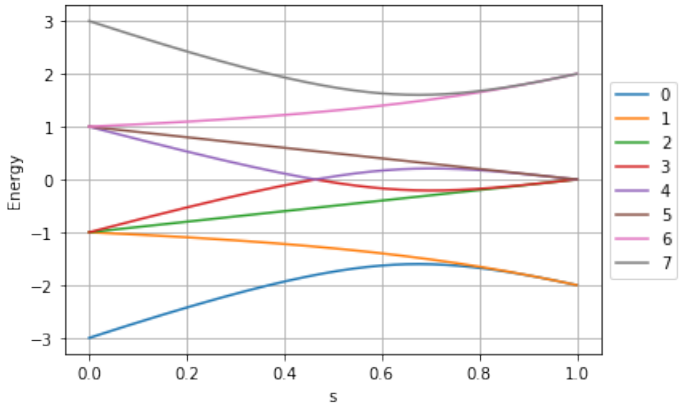

Figure 1: Complete spectrum for N=3, 1000 steps, $\lambda_1 = \lambda_2 = 1$.

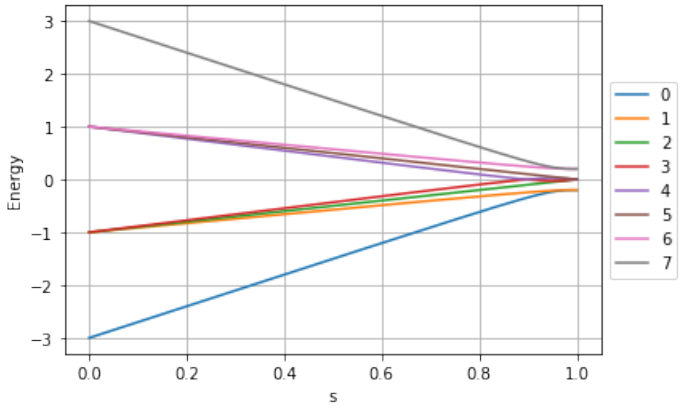

Figure 2: Complete spectrum for N=3, 1000 steps, $\lambda_1 = \lambda_2 = 0.1$.

As we can see, the first two spectra look quite different; in particular, for our purposes, the most important thing to notice is that the energy gap between the states, in particular at the end of the interval, is much smaller for the smaller values of λ. This is not surprising: as discussed in Sec.2 smaller interactions lead to smaller energies, and so to smaller gaps between the levels. Later on we will see how this affects the estimator of Eq.6. From the third graphic

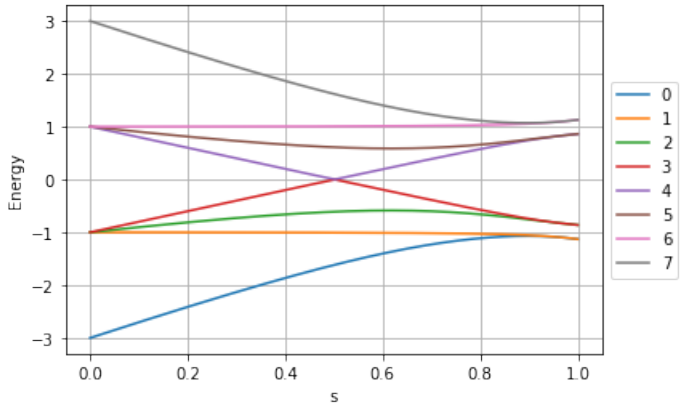

Figure 3: Complete spectrum for N=3, 1000 steps, $\lambda_1 \sim 0.995, \lambda_2 \sim 0.134$.

we can see, instead, that the presence of the random field breaks the degeneracy between some higher values at the end of the spectrum, but not the one of the ground state present at the final instant, as expected. Unfortunately, it doesn't avoid the crossing between the third and the fourth level; this situation is found for the bigger systems also.

Let's now examine the parity, that was checked by computing the expectation value of the parity operator on each state at each time step: the result is shown in Fig.4. As ex-

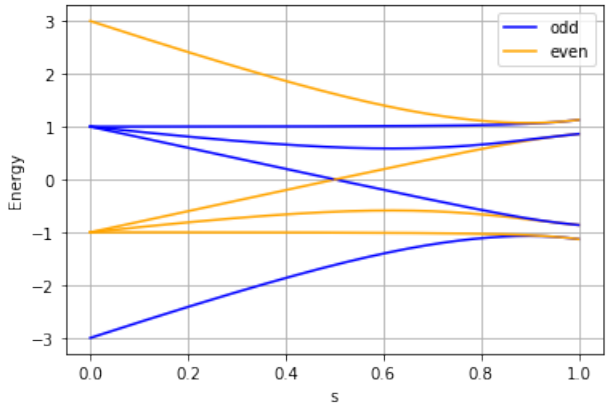

Figure 4: Complete spectrum computed for N=3 and 1000 steps, with the parity of the relative states in evidence.

pected from Eq.11, each state keeps its parity for the whole evolution. As it can be seen, the first state for which ϵ_i will be not null is the fourth; after the level crossing that happens at $s \sim 0.5$ one must be careful, because it becomes the third.
The whole spectrum computed allows us to calculate ϵ, g and the estimator; the results about these three quantities as a function of the fractional time s are shown in Figg.5,6,7

As expected the quantity ϵ is zero for all the even states, and it is possible to see the consequence of the crossing between the third and the fourth state. The gap has been computed only for the cases of interest; as expected it becomes smaller (and then, "dangerous") at the end of the evolution. The

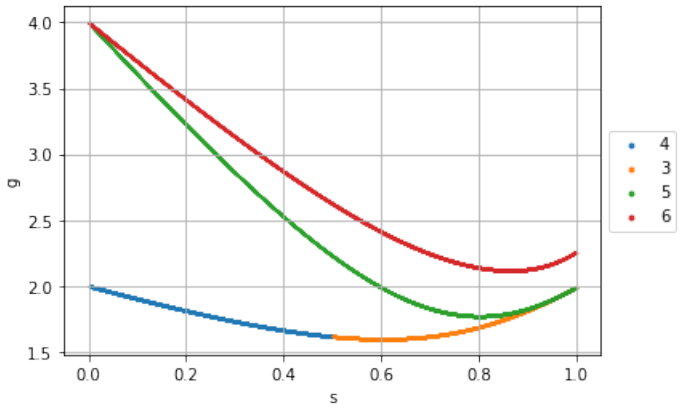

Figure 5: Gaps between the ground state and the other odd states at N=3, 10000 steps.

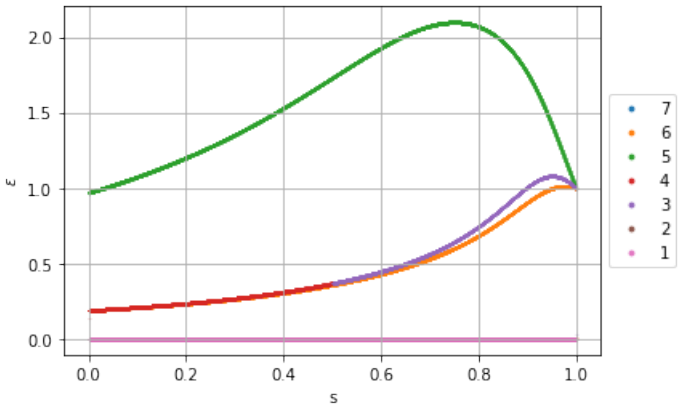

Figure 6: ϵ between the ground state and all the others at N=3, 10000 steps.

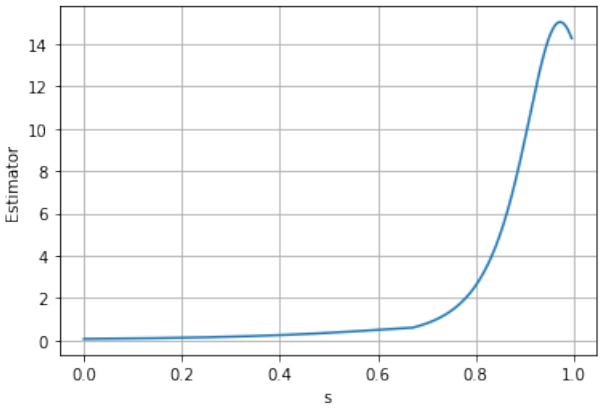

Figure 7: Estimator for N=3, 10000 steps.

estimator is computed using Eq.7: it is very peaked at the end, because of the nearness between the ground state and the third excited. The maximum has been computed, and the condition for applying our adiabatic quantum computation is:

$$T \gg\sim 15\,. \tag{17}$$

In order to study the reliability of the inequality, the evolution has been performed for several values of T, each with 100000 steps: the very low size of the system let the program complete all the calculations with this input value in few seconds.

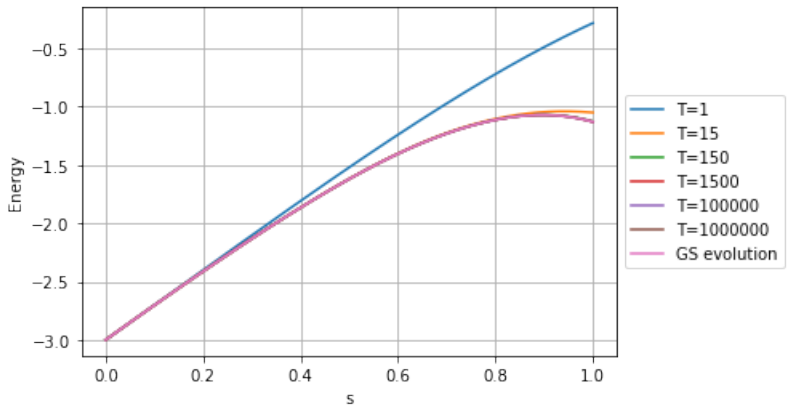

Figure 8: Time evolution for some values of T and "real" ground state evolution for N=3, 100000 steps.

The lines shown in Fig.8 give a first confirm of our hypothesis: while for $T = 1, 15$ the evolution clearly doesn't match the "real" evolution, for $T = 10, 100$) and more times bigger the evolution is indistinguishable from the "real" one. In Fig.9 are shown the evolutions for the largest values of T at the final instants, and in Tab.1 are collected the the parameters $\Delta t = T/(\#\text{ of steps})$ and the error σ, that is defined as the difference between the evolution and the "real" evolution at the final instant.

T	Δt	σ
1	$1{\cdot}10^{-5}$	0.85
15	$1.5{\cdot}10^{-4}$	0.079
150	$1.5{\cdot}10^{-3}$	$0.34{\cdot}10^{-3}$
1500	$1.5{\cdot}10^{-2}$	$0.53{\cdot}10^{-4}$
$1 \cdot 10^5$	1	$0.11{\cdot}10^{-4}$
$1 \cdot 10^6$	10	$0.11{\cdot}10^{-4}$

Table 1: Evolution results for N=3, 100000 steps.

As it can be seen, a T one thousand times bigger than the estimator leads to an error one order of magnitude smaller than a T "only" one hundred times bigger than the estimator, and the result can be considered as satisfactory. Increasing T even more doesn't lead to a significant decrease of the error; on the other hand it is surprising to not to see the evolution completely miss the task, by the moment that

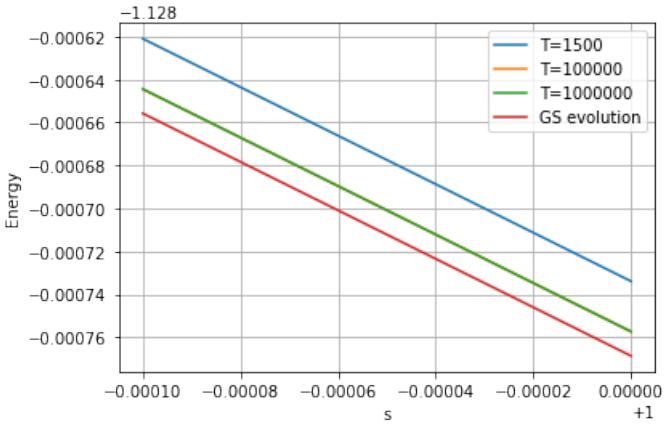

Figure 9: Final instants of the time evolution for the biggest values of T and "real" evolution, N=3, 100000 steps.

Δt, that is related to the error of the algorithm, becomes very big.

Finally, we have to recall that the gap between the states strongly depends on the various lambdas. To analyze the problem, the estimator was calculated for all the possible pairings of the two $\lambda \in [-1, 1]$, with a spacing of 0.1. The result is shown in Fig.10.

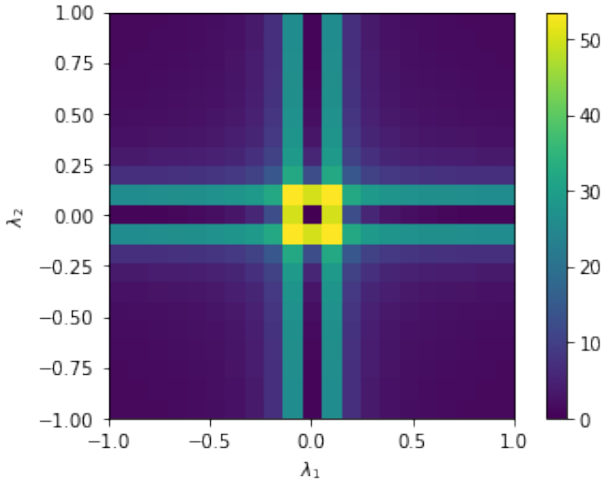

Figure 10: Value of the estimator for N=3, for a grid of lambdas spaced by 0.1 in $[-1, 1]$

The figure is symmetric: the sign of the lambdas doesn't affect the problem, while the values of the two lambdas strongly affect the estimator, that can have a value close to one, or even bigger than 50. This important result gives us an idea about the difficult of performing the adiabatic quantum computing in the "unluckiest" cases.

5 Eleven particles

With eleven particles the study of the system becomes complicated because of the limits of the computational efficiency: here, one iteration of the subroutine that diagonalizes the matrix for computing the whole spectrum takes almost three minutes, that means five hours for one hundred steps. An attempt was made to study a system made of $N = 12$ particles, but more than 16 hours would have been needed only for the complete spectrum for 100 steps.

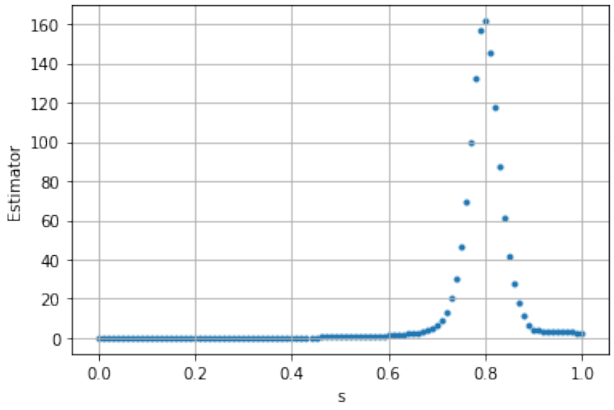

Figure 11: Estimator for N=11, 100 steps

As it was seen in the previous section, there is no need of a very precise estimation of the estimator, by the moment that T has to be set orders of magnitude bigger than it. Hence, it was retained enough to compute the estimator only for 100 steps (Fig.11), and without making a further analysis in the interval around the maximum (e.g. $[0.75, 0.85]$). The result, for the randomly generated configuration reported in Tab.2 is:

$$T \gg\sim 161.5\,. \tag{18}$$

At this point the evolution was made, setting $T = 16150$

λ_1	0.995
λ_2	0.134
λ_3	0.932
λ_4	0.496
λ_5	-0.265
λ_6	$-0.387 \cdot 10^{-1}$
λ_7	-0.852
λ_8	-0.989
λ_9	-0.306
λ_{10}	-0.316

Table 2: Random extracted lambdas for the N=11 analysis.

with 1615 steps. With this number of steps, the algorithm took about six hours to finish; unfortunately the author was unable to do more: choosing a number of steps just an order of magnitude bigger, would have committed his only pc for about sixty hours. The result is shown in Fig.12, and the final error estimated is

$$\sigma \approx 0.14\,. \tag{19}$$

The result can't be considered satisfactory: as we have seen for the $N = 3$ case, the error can be made much more smaller setting higher values of T. On the other hand, T can't be

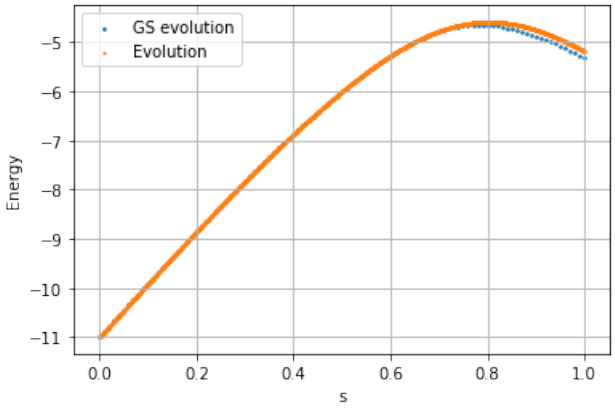

Figure 12: Time evolution and "real" ground state evolution for N=11, T=16150, 1615 steps.

increased "for free" to obtain better results: the computational cost lies in the number of steps, that must be increased if T is increased, in order to have Δt small. The results shown in Fig.13 (obtained with the same number of steps but with $T = 161500$) clearly show the problem. Here

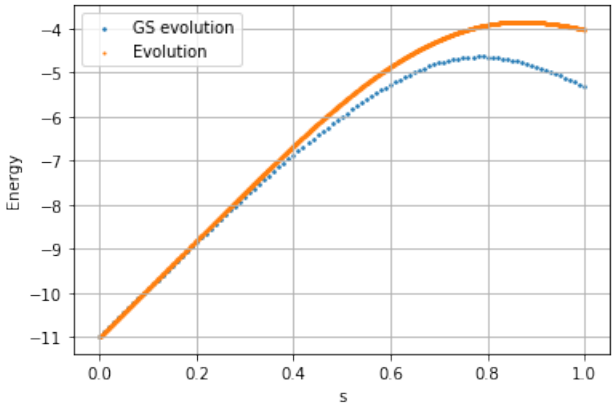

Figure 13: Time evolution and "real" ground state evolution for N=11, T=161500, 1615 steps.

the error is

$$\sigma \approx 0.13 \cdot 10\,. \tag{20}$$

6 Application: codification of classical hard problems in a quantum spin Hamiltonian

Ising spin glasses are known to be NP-hard problems for classical computers, so it is natural to suspect intimate connections with all other NP problems: an NP-hard problem is an optimization problem (what is the ground state energy of H?) [1]. There are several class of problems that can be codified as the Hamiltonian of an Ising spin glass; here, just to make a practical example, we will study the partitioning problems.
Number partitioning asks the following: given a set of N positive numbers $S = \{n_1, \dots, n_N\}$, is there a partition of this set of numbers into two disjoint subsets R and $S - R$, such that the sum of the elements in both sets is the same? [1] This can be phrased trivially as an Ising model as follows. Let $n_i (i = 1, \dots, N = |S|)$ describe the numbers in set S, and let

$$H = \left(\sum_{i=1}^{N} n_i s_i \right)^2 \tag{21}$$

with $s_i = \pm 1$ a classical Ising spin variable [1]. It is clear that if there is a solution to the Ising model with $H = 0$, then there is a configuration of spins where the sum of the n_i for the $+1$ spins is the same for the sum of the n_i for the -1 spins. Thus, if the ground state energy is $H = 0$, there is a solution to the number partitioning problem [1]. Additionally, we retain that these problems can be codified also with a quantum Ising model, e.g. by taking

$$\hat{H} = \sum_{i=1}^{N} \sigma_z^i n_i \tag{22}$$

and again verifying if the ground state is zero. If it is, then the respective eigenstate can be found, i.e. the direction of the spins along the $\hat{z}$ axis, i.e. the partitioning configuration. Finally, a note about the degeneracy: the eventual null ground state would have for sure degeneration two: found a solution, the other one is found simply by flipping all the spins of the first; this just resemble the fact that one can swap the content of the subset S with the content of the subset $S - R$, and obviously have the same partition. The degeneracy can be avoided by fixing one of the spins, and hence solving the problem for the remaining $N - 1$ ones [1].

7 Further work

The slowness of the algorithm didn't allow to perform a more detailed analysis for the bigger systems: both a more complete analysis of the system and of the efficiency of the algorithm are topics of interests. Furthermore, a more complete analysis about the dependence of the estimator on the lambda values could be performed, in order to have an idea of the computational complexity for a system of generic dimension N.

References

[1] A. Lucas, Ising formulations of many NP problems, https://doi.org/10.3389/fphy.2014.00005, 3-24 (2014).

[2] Tameem Albash, Daniel A. Lidar, Adiabatic quantum computation, Rev Mod Phys. , **90**, 517–527, 533-537 (2018).