Quantum Annealing in the transverse Ising Model

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(Dated: June 12, 2018)

Abstract: In this work we perform numerical simulations of a quantum annealing procedure to find the ground state of a target Hamiltonian. By using this technique one starts from an Ising Hamiltonian with a transverse field that forces the spins to point in the x direction. The field is removed slowly with time, the purpose of this is to carry an adiabatic transition from the transverse-field Hamiltonian to the target Hamiltonian. In order to prove the functionality of quantum annealing we will introduce two terms to quantify the success of the protocol.

I. INTRODUCTION

Many NP-complete and NP-hard problems can be reduced to that of finding the ground state of a complex system of spins with global interaction [1]. When the size of the system is large and direct computation is no longer possible, quantum annealing has proven to be an effective heuristic method for finding the solution. Quantum Annealing (QA) was proposed as an alternative to Simulated Annealing (SA) by Kadowaki and Nishimori [2]. As they said in their original paper, unlike SA in which transitions between states occur due to thermal fluctuations they 'introduced quantum fluctuations into the simulated annealing process of optimization problems, aiming at faster convergence to the optimal state' [2]. It was tested by the quantum version of the Ising model and they proved that this technique was successful with larger probabilities than SA in the same conditions.

QA has been growing in importance since its proposal and nowadays companies such as D-Wave and IBM are working on building an effective quantum annealer. Seven years ago, in 2011, D-Wave launched its first commercial quantum annealer on the market, 4 years later, in 2015, Google announced [3] that the D-Wave quantum annealer outperformed both SA and Quantum Monte Carlo on a set of hard optimisation problems. While results like this are encouraging we are still far from turning QA into a practical technology. Moreover, notice that a quantum annealer is not a traditional quantum computer, it does not work as a quantum Turing machine and therefore cannot execute quantum algorithms such as Shor or Grover. Despite its limitations the benefits that QA can bring to society are many, some of its applications include fields like medicine, urbanism and communications [4].

Our main objective in this work will be to understand how QA works using a numerical simulation of the process for a small number of spins and test whether QA can be used to find the ground state of a complex Hamiltonian.

This work is organised in the following way. In section II we introduce the theoretical model and define the annealing procedure. Then, in section III, we explain the procedure we followed in order to solve the time-dependent Schrödinger equation (TDSE). Before presenting our results in section IV, we introduce two different ways to quantify the success of the annealing protocol. Finally, our results will be presented and discussed, the work will conclude in section V where we provide a brief summary and the conclusions drawn from our work.

II. THE MODEL

We consider a quantum version of the one dimensional Ising model. The Hamiltonian of the system is written as:

$$\mathcal{H}(t) = \mathcal{H}_0 - \Gamma(t) \sum_i \sigma_i^x \ ,$$

where

$$\mathcal{H}_0 = -\sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z - \alpha \sum_i \sigma_i^z.$$

To simplify notation we have set $\hbar = 1$ and all magnitudes are taken as adimensional, σ^z and σ^x are the 2x2 Pauli matrices. The target Hamiltonian, $\mathcal{H}_0$, has two different parts. First, an Ising Hamiltonian with a complex pattern of couplings, J_{ij}. The small longitudinal field is introduced to break the spin degeneracy, we set $\alpha = 0.1$. The transverse field in $\mathcal{H}(t)$ plays the same role in QA as the temperature in SA, since $[\sigma^z, \sigma^x] \neq 0$ quantum tunneling between states will occur as the system evolves. To ensure that the problem is difficult we choose an all to all coupling with random numbers. Thus, J_{ij} is chosen from a Gaussian distribution of mean 0 and $\sigma_E = 1$.

In our case, as we will work with a small number of spins on the σ^z basis, $\mathcal{H}_0$ is directly diagonal and we can find the target ground state by simple means. But, for instance, if we had a system with 50 spins, the Hilbert space is 2^{50} and one cannot find the ground state so easily. Thus, in this work the ground state of the target Hamiltonian $\mathcal{H}_0$ is known and therefore we will be able to test the accuracy of the annealing protocol.

The annealing protocol is defined in the following way. At $t = 0$ we will choose $\Gamma(0)$ large enough such that the

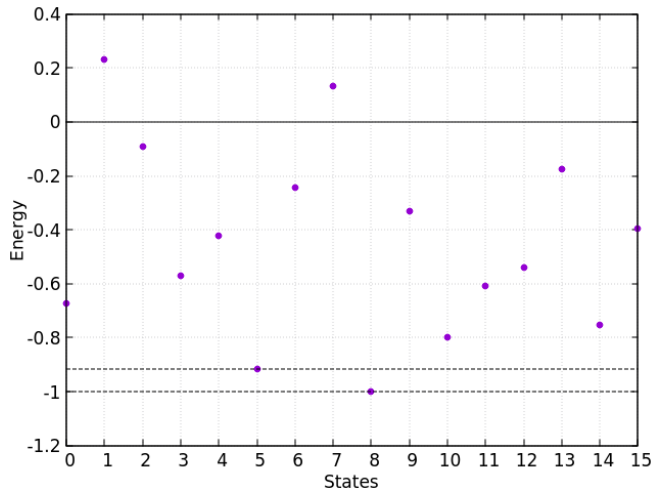

Figure 1: Energy landscape of a system with 4 spins and a single ground state in the eight state, which corresponds with the pattern $\left|\phi^0_{gs}\right\rangle \equiv |\downarrow\uparrow\uparrow\uparrow\rangle$, and a gap $E_g = 0.0812$.

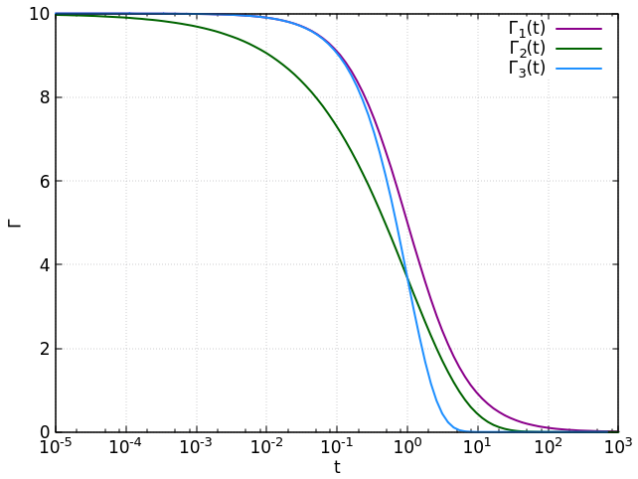

Figure 2: Annealing protocols considered in this work.

ground state of the $\mathcal{H}(0)$ is, with good approximation, the state $|+\rangle\,|+\rangle\,...\,|+\rangle$ which is an equal probability superposition of all states in the σ^z basis, being $|+\rangle$ the eigenvector that $\sigma^x\,|+\rangle = |+\rangle$. As time evolves $\Gamma(t)$ will go from the initial large value to approximately 0. In this way and according to the Adiabatic Theorem, if we make the transition slow enough and there is a significant gap between the ground state and the first excited state the evolved state will be essentially the instantaneous ground state for any t. Even when the adiabatic conditions are not met we can still obtain the right pattern of average spins, which can be thought of as a way of measuring the quality of the protocol.

III. THE METHOD

A. Solving time-dependent Schrödinger equation

The dynamics of the system is governed by the TDSE which in natural units reads:

$$i\frac{\partial\,|\phi(t)\rangle}{\partial t} = \mathcal{H}(t)\,|\phi(t)\rangle\,. \tag{1}$$

The initial state is taken to be the ground state of the Hamiltonian at $t = 0$. This is obtained by numerically diagonalising the full Hamiltonian. Note this initial state is approximatelly the $|+\rangle\,|+\rangle\,...\,|+\rangle$ state. To solve the time-dependent Schrödinger equation we can derive the Crank-Nicolson algorithm in the following way. We can approximate $|\phi(t+\Delta t/2)\rangle$ in two different forms: as the next semi-step of the current $|\phi(t)\rangle$ or as the previous semi-step of an advanced $|\phi(t+\Delta t)\rangle$.

This can be written as:

$$|\phi(t+\frac{\Delta t}{2})\rangle = (1 - \frac{i\Delta t}{2}\mathcal{H})|\phi(t)\rangle\ , \tag{2}$$

$$|\phi(t+\frac{\Delta t}{2})\rangle = (1 + \frac{i\Delta t}{2}\mathcal{H})|\phi(t+\Delta t)\rangle. \tag{3}$$

Now we equal (2) and (3), and isolate $|\phi(t+\Delta t)\rangle$ to find

$$|\phi(t+\Delta t)\rangle = \left(1 + i\frac{\Delta t}{2}\mathcal{H}\right)^{-1}\left(1 - i\frac{\Delta t}{2}\mathcal{H}\right)|\phi(t)\rangle. \tag{4}$$

Libraries already implemented in Python provide functions to diagonalise, compute the inverse matrix and handle matrix products. Before going into further details it should be mentioned that the consistency of the method has been tested for different values of Δt.

B. Measures of the quality of the protocol

Once $|\phi(t_f)\rangle$ is obtained we will evaluate the quality of the annealing mainly in two ways: by computing $|\langle\phi(t_f)|\phi^0_{gs}\rangle|^2$ to find the overlap between the evolved state and the target state $\left|\phi^0_{gs}\right\rangle$ (a value of 1 would be a complet success), by computing expected value of spin for every site $\langle\sigma^z_i(t_f)\rangle$. We will be also interested in comparing eigenvalues with the average energy $\langle\mathcal{H}(t)\rangle$ and its variance σ^2_E during the transition. Diagonalising we will find instantaneous eigenvalues and eigenvectors that will be used to compute $|\langle\phi_{gs}(t)|\phi^0_{gs}\rangle|^2$, the pure adiabatic path. Of the two ways presented to quantify the success of the annealing notice that overlap is not an observable. Since in an experimental setup we will be measuring the spin for every site, it becomes relevant to evaluate the annealing in terms of an observable such as the pattern $\langle\sigma^z_i\rangle$. Hence, another way of quantifying the success of the annealing protocols is by defining a Fidelity measure as in [5]:

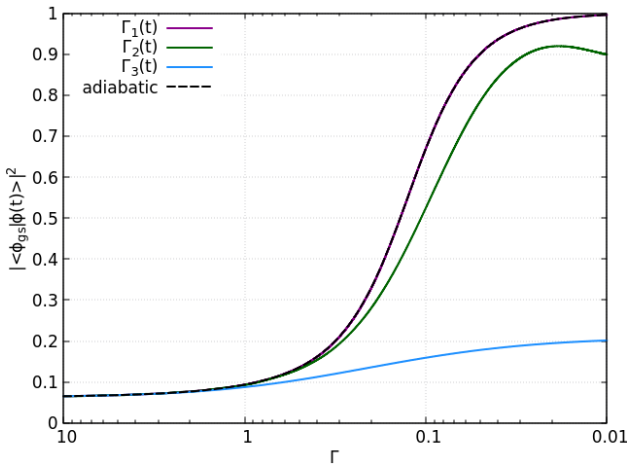

Figure 3: Overlap between the evolved state and the ground state of the target Hamiltonian for the three different protocols. The exact adiabatic path is also depicted in dashed lines, almost coinciding with the slow protocol Γ_1.

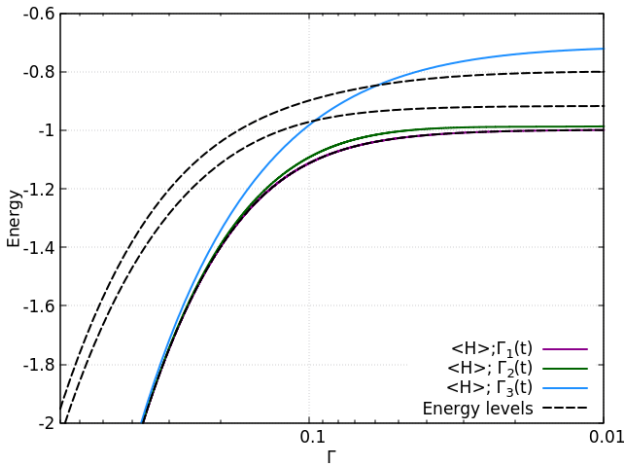

Figure 4: Comparison between the instantaneous low energy eigenvalues of the Hamiltonian, dashed lines, and the average energy of the Hamiltonian with the three different protocols.

$$F = \begin{cases} \min|\langle\sigma_i^z(t_f)\rangle| & \text{if sign of } \langle\sigma_i^z(t_f)\rangle \text{ is correct } \forall \text{i.} \\ 0 & \text{Otherwise.} \end{cases} \tag{5}$$

This definition gives 0 if the signs of the spins at the end of the protocol do not coincide with those of the ground state of $\mathcal{H}_0$. If the sign pattern is reproduced, we get a positive fidelity.

IV. NUMERICAL RESULTS

We have considered three functional forms for $\Gamma(t)$: $\Gamma_1 = 10/(t+1)$ as an example of slow transition, $\Gamma_2 = 10/e^{\sqrt{t}}$ as an intermediate case and $\Gamma_3 = 10/e^t$ as a model of fast transition. They are depicted in Figure 2. In all cases we will start at $t = 0$ from the same value of $\Gamma(0) = 10$ and stop the evolution when we reach the final value, $\Gamma_f = 0.01$. Since the duration of the process depends on the Γ we are testing, when we look into the differences between faster or slower transitions we will plot magnitudes as a function of Γ rather than time. In this way we emphasize the fact that depending on the actual functional form we do get different results for the same value of Γ.

A. Single realisation

First, we will discuss how different annealing protocols work for one specific realisation of the random couplings J_{ij}. In this way, we will get familiar with the main concepts used to characterize the annealing protocol. We will consider a system of 4 spins, which can be simulated extremely fast with current computers. The energy landscape of the problem is given in Figure 1, that is, we depict in the figure all the eigenvalues of the target Hamiltonian. For instance, in this specific case the ground state of the system corresponds to the pattern $\left|\phi_{gs}^0\right\rangle = |\downarrow\uparrow\uparrow\uparrow\rangle$.

In Figure 3 we depict the first indicator of the quality of the protocols, the overlap between the evolved state and ground state of the target hamiltonian. As expected, the faster the Γ the worse the final overlap we obtain with the protocol. In the figure we are comparing the three evolutions with the actual adiabatic result. In this way, we can clearly see that the evolution with Γ_1 is essentially adibatic, providing a final overlap of the order of 1. With Γ_2 we depart from adiabaticity, the final overlap is now 0.9. The exponential ramping, being the fastest of all, produces the worst final overlap, of just 0.2.

To better understand how the annealing protocol works we will study the instantaneous excitation of the excited modes. A way to see this is to compare the average energy of the evolved state, with the instantaneous ground state energy and lower excitations. This is obtained by direct diagonalisation of $\mathcal{H}(t)$ at different values of Γ. Note this comparison could not be made in a realistic case with more than 50 spins.

The slow protocol Γ_1 clearly produces an evolution where the average energy always falls on top of the instantaneous ground state energy, thus producing an adiabatic evolution, see Figure 4. The intermediate case, Γ_2, excites some low energy modes of the instantaneous Hamiltonian, and thus the average energy is found to be larger, as seen in Figure 4. On the other hand, the fast protocol produces large mixing with the first excitations of the instantaneous Hamiltonian, as in particular at the final value of Γ, produces an average energy above the second excited state, clearly departing from the adiabatic result. Figure 5 reveals why the slow transition produces such a good overlap compared to Γ_2, as

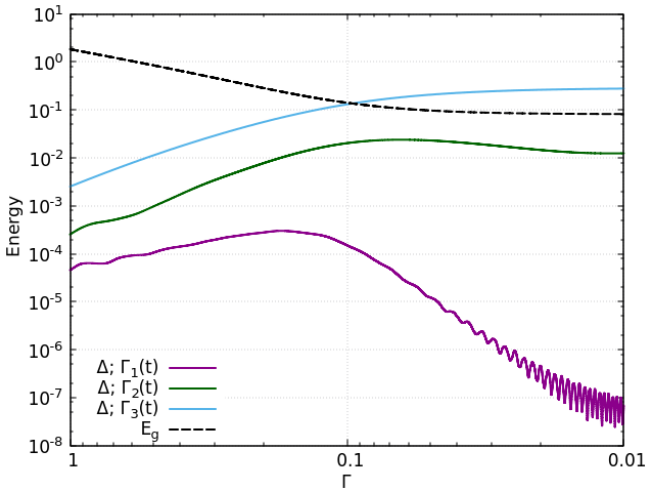

Figure 5: Instantaneous excitation energy gap, dashed line, compared to the evolved excitation energy $\Delta \equiv \langle \mathcal{H}(t) \rangle - E_0$, computed for the three protocols considered.

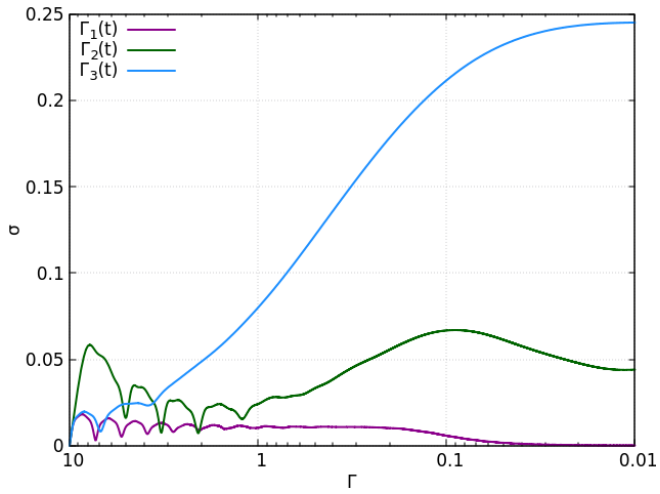

Figure 6: Standard deviation of the energy of the evolved state, computed as shown in (6), for the three protocols described in the text.

we slowy switch off the field and quantum tunneling between states becomes less likely, the difference between the expected value of energy for Γ_2 turns out to be 10^5 times bigger than the same for Γ_1.

From another point of view, an adiabatic transition means that the evolution takes place from an eigenstate of $\mathcal{H}(t)$ to the corresponding eigenstate of $\mathcal{H}(t + \Delta t)$. If the wave function gains components of other states means that we are not longer in an eigenstate of $\mathcal{H}(t)$. This can be measured by the standard deviation

$$\sigma_E = \sqrt{\langle \phi(t) | \, \mathcal{H}^2(t) \, | \phi(t) \rangle - \langle \phi(t) | \, \mathcal{H}(t) \, | \phi(t) \rangle^2} \,, \quad (6)$$

which is null when we are in an instantaneous eigenstate of the Hamiltonian and positive otherwise. In Figure 6 we see the evolution of the standard deviation for the three annealing protocols for the same coupling pattern which gives rise to the landscape in Figure 1. It is interesting to notice that, as we can check in Figure 2, the slope of Γ_2 is steeper than the one of Γ_3 for small t. This is reproduced in Figure 6 where we can see that, at the beginning of the annealing, the initial states corresponding to the Γ_3 ramping are closer to eigenstates than those related to Γ_2.

As mentioned, the overlap defined above is not the only indicator of the success in the annealing protocol. In fact, it is more useful to define an observable that can quantify the success of the protocol. In section III we introduced a fidelity with this purpose. For instance, in Figure 7 where the evolution of $\langle \sigma^z \rangle$ is shown for the four sites in the system, fidelity would be the last $\langle \sigma^z \rangle$ of the 3rd site. Obtaining the correct pattern of spins even for fast transitions is satisfactory, but should also be considered that with such low probabilities one could measure the wrong spin in one site and would not know. In conclusion, Figure 7 shows that the method is robust but not flawless.

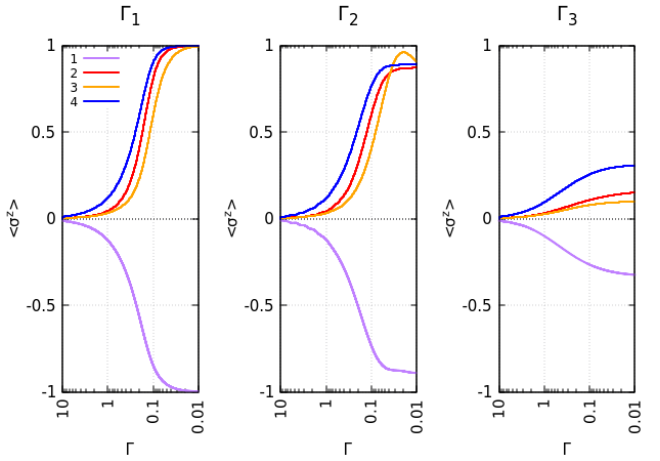

Figure 7: Evolution of $\langle \sigma^z \rangle$ for each of the 4 spins in the chain. In this case even for exponential ramping we obtain the right pattern of spins, which is remarkable and it is not the general case.

B. Averaging for multiple realisations

Everything that has been mentioned such as overlap, eigenvalues and fidelity are particular for every realisation. This means that every different choice of J_{ij} will yield a different energy landscape and hence a different behaviour. Therefore it is interesting to compute the mean values of overlap and fidelity plus its deviation over a large number of realisations so we can have a broader view on the phenomena. In Figure 8 is shown the mean evolution of the overlap for each protocol for 1000 realisations with different J_{ij}. As we see in Figure 8, there is little variance in the behaviour, we can infer that Γ_1 is slow enough (in our time-scale) to almost guarantee that

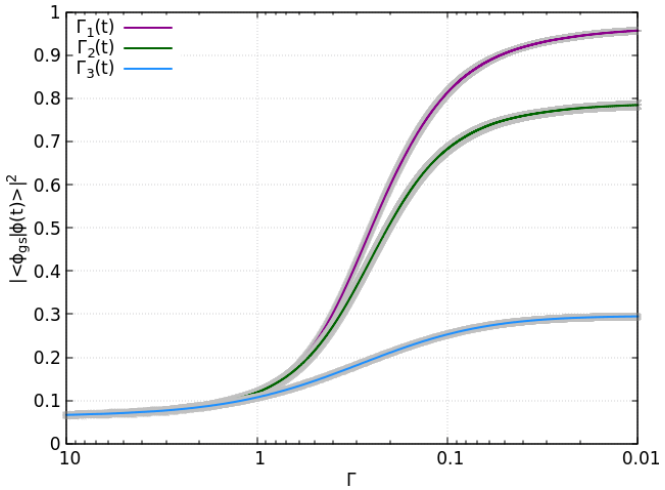

Figure 8: Mean overlap for 1.000 different realisations for each protocol and its standard deviation, shady outline.

	Γ_1	Γ_2	Γ_3
Mean Fidelity	0.935(6)	0.640(10)	0.114(3)

Table I: Mean fidelities for each protocol with 1.000 different realisations.

we will measure the ground state when the annealing is complete. The mean fidelities provide a similar picture. As we can see in Table I we get large average fidelity for Γ_1, a smaller value for Γ_2 and a very small fidelity for Γ_3.

But again, since the process is affected by the particular conditions of every landscape (this is, of every particular problem we are solving) we cannot be secure of what protocol we need to use to ensure the success of the annealing.

V. SUMMARY AND CONCLUSIONS

In this work we have studied the ability of QA protocol to find the ground state of a target Hamiltonian. The target Hamiltonian is chosen to be "difficult" in the sense that small gaps and many local minima may appear depending on the realisation. We have done this by making the interaction coefficients J_{ij} random following a gaussian distribution with vanishing mean and standard deviation 1. The protocol is performed by turning off a transverse field in a controlled way. We have presented two ways of evaluating the quality of the protocol; 1) To compute the overlap between the target state and the one obtained after the evolution, 2) By comparing the average spin pattern after the evolution. The second method is prome to experimental implementation as it accounts to measuring the average spin at each site. We averaged both of them for a large number of iterations for different protocols and we found that it is a robust and efficient method to find the ground state. In summary:

(i) Quantum Annealing works very well for slow varying $\Gamma(t)$, as expected from the adiabatic theorem. For fast ramping, however, we do find that even though the overlap may not be very large, the average spin pattern is correctly reproduced.

(ii) Due to the probabilistic nature of the process there will always be some uncertainty in the solution that the annealer yields. Adiabaticity plays a fundamental role in the process and needs to be carefully addressed in an experimental quantum annealer.

Our study has been done with 4 spins but we have also performed some computations with 8 spins and the qualitative picture is the same. Working with a larger number of spins means a much larger Hilbert space for the system, this will bring a more complex energy landscape that involves more local minima and lower gap. As a consequence, we will usually need slower protocols to achieve the same results they would produce on a smaller system.

Acknowledgments

We want to thank B. Julià-Díaz and A. Polls for all the time and dedication, without the useful discussions we had this work would not have been possible. Also a special mention to J.Cid, family and friends for their support, that came in many ways.

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