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Dynamics of Quantum Annealers: Ising Model with Transverse Field Study

A. Więckowski[a,*] and A. Ptok[b]

[a] *Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology, PL-50370 Wrocław, Poland*
[b] *Institute of Nuclear Physics, Polish Academy of Sciences, ul. W.E. Radzikowskiego 152, PL-31342 Kraków, Poland*

Doi: 10.12693/APhysPolA.138.686 *e-mail: andrzej.wieckowski@pwr.edu.pl

Quantum computers can be a big step towards a further advancement of our technology. There is already an available generation of the first adiabatic quantum annealers. The crucial question is how quantum and how adiabatic these prototypes are. We study the dynamics of the quantum Ising chain and investigate different quantities. We discuss probabilities of obtaining correct results from the exact dynamics via the Landau–Zener formula concerning the annealing procedure.

topics: Landau–Zener transition, quantum annealing, Ising model

1. Introduction

Computers are probably the most important inventions in the history of mankind. They can be found in every aspect of our life. They can help us, support us or even save our lives. However, we are still trying to improve the performance of computers to do better and faster calculations with lower energy consumption.

We must have in mind that modern progress in CPU development is limited by famous Moore's law [1]. In fact, probably around 2020, this law will not be working anymore [2] due to greater miniaturization of integrated circuits, reaching the limit of quantum scales. This fact starts a discussion about the realization of quantum computers.

It is highly probable that we owe the early development (the main idea) of quantum computing to these three scientists and their corresponding works: Paul Benioff [3], Yuri Manin [4] and Richard Feynman [5]. Then, some progress has been achieved. People developed algorithms for some problems which had better performance than any other algorithm which could be performed on classical computers. Most of the quantum algorithms are probabilistic. A successful final result is obtained with a huge probability. In contrast, most algorithms on classical computers are deterministic which means that one has a 100% probability of success (on a reliable machine).

A real race began in 1998, when the first realization of Grover's algorithm was performed on a two qubits system [6]. Over the last 20 years, huge progress has been made. After this time, technology has made some progress too. The three big companies, IBM, Google and Intel, own universal quantum computers ranging from 49 to 72 qubits [7]. The first commercial quantum computing company, i.e., D-Wave Systems, has in its offer 2048-qubit adiabatic quantum computers using quantum annealing. The next quantum computer with 5000 qubits has already been announced [8, 9]. In this work, we will study theoretical aspects of quantum computing based on the quantum annealing method, similar to the ones used in D-Wave's machines.

Adiabatic quantum computing (AQC) is a computational model [10–12] which can solve any problem a universal quantum computer (gate model) should be able to solve (maximally with some polynomial-time penalty) [13]. AQC relies on the adiabatic theorem which says that if a system in an n-eigenstate (especially ground state) of the initial Hamiltonian $\hat{H}_i$ evolves adiabatically in time to the final Hamiltonian $\hat{H}_f$, it will remain in the n-eigenstate. The first proof of this theorem was given by Fock and Born [14, 15] in 1928. The main problem with AQC, in fact, is to determine whether its evolution is adiabatic, i.e., how slowly one should perform quantum dynamics. For this purpose, we test adiabaticity using different quantities. Additionally, we demonstrate the application of the Landau–Zener formula. The main objective of this paper is to compare the exact quantum evolution of the simple annealing problem to the analytical Landau–Zener solution. The paper is organized as follows: the general problem is described in Sect. 2, the model and methods description are given in Sect. 3, our results are presented in Sect. 4 and summarized in Sect. 5.

2. Quantum annealing

Qubits in D-Wave machines are connected via chimera topology. A part of complicated connections (couplers) structure is presented in Fig. 1. Units are connected in such a way that vertical/horizontal qubits are connected with neighbouring vertical/horizontal qubits (colored with green/red). Since such a system is a finite system (with an open boundary condition), some of the units have only 2 or 3 neighbours (but not 4), see Fig. 1. These units are certainly located on the grid edge. However, not all connections between qubits are available. One should properly embed studying the case into such a topology where qubits resource is sufficient. The embedding of more complex problems, e.g. the ones which require high connectivity graphs, may not be possible.

The main idea of AQC is based on the adiabatic theorem. First, the initial state is started from an easy initial Hamiltonian $\hat{H}_i$ ground state. Then, the system is evolved on some path associated with function $f(\tau) \in [0,1]$, $f(-1) = 1$, $f(1) = 0$, $\tau \in [-1,1]$ into a ground state — due to the adiabatic theorem — of a final, desired Hamiltonian $\hat{H}_f$. The final Hamiltonian is constructed in such a way that it should produce the correct answer for a specific problem included in the ground state. Therefore, the time-dependent Hamiltonian of system $\hat{H}(\tau)$ can be written in the following form:

$$\hat{H}(\tau) = f(\tau)\hat{H}_i + [1 - f(\tau)]\,\hat{H}_f, \tag{1}$$

where $\tau = t/T$ is the normalized time, t is the time and T is the annealing time (half of the total evolution time).

Quantum annealing (QA) is a heuristic method for solving optimization combinatorial problems [11, 16–23]. Most of these tasks belong to the NP-hard complexity class. Alternatively, QA can be considered as a physical (or simulated) realization of some algorithms from AQC. QA owes its name to simulated annealing (SA). In some way,

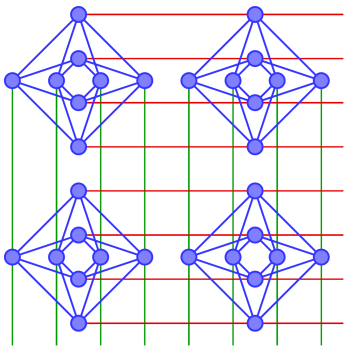

Fig. 1. Schematic representation of the chimera graph topology realized on D-Wave machines. Circles represent qubits (in practice realized by SQUIDs), while lines correspond to possible couplings between them.

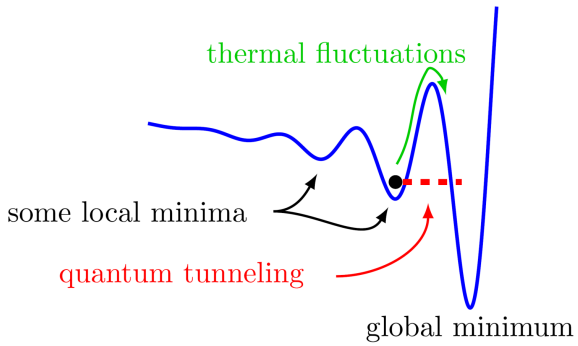

Fig. 2. A schematic view of the difference between the mechanism of simulated annealing and quantum annealing.

it is a precursor of QA. Simulated annealing is a technique for global optimization of some function that, e.g., finds a minimum. The inspiration for this method was annealing (heat treatment) in metallurgy. The algorithm starts from a random state of the problem. Next, one tries to alter the state slightly. Then, some quantity of a current state is measured and a decision if a newly modified state is accepted or not is made with some probability (depending on temperature). In the next steps of the algorithm, temperature is decreased to a sufficiently low limit, so with some probability at each step, there is a chance that the state will become worse than in the previous iteration. This is very important and purposeful because it prevents stacking at local minima. It can be compared to thermal fluctuations which move the system in a potential landscape in the direction of global minima (Fig. 2). In contrast to thermal fluctuation in SA, quantum fluctuations are used in QA.

3. Model and method

In general, evolution of a quantum state $|\psi\rangle$ of the system that is described with a Hamiltonian $\hat{H}$ is given by the equation of motion, i.e., the time-dependent Schrödinger equation (TDSE) [24],

$$\mathrm{i}\hbar\partial_t|\psi\rangle = \hat{H}|\psi\rangle. \tag{2}$$

Further, we assume $\hbar = 1$. In the case of time-independent Hamiltonians, one can solve (2) by finding eigenstates of $\hat{H}$, based on the time-independent Schrödinger equation (TISE):

$$\hat{H}|n\rangle = E_n|n\rangle. \tag{3}$$

In case of D-Wave's machines, they can be considered as a physical realization of the Ising model with a transverse field [11, 23, 25–27], described by the given time-dependent Hamiltonian $\hat{H}$:

$$\hat{H}(\tau) = -A(\tau)\sum_{i=1}^{L}\Delta_i\sigma_i^x - B(\tau)\left(\sum_{\langle i,j\rangle}J_{ij}\sigma_i^z\sigma_j^z + \sum_{i=1}^{L}h_i\sigma_i^z\right), \tag{4}$$

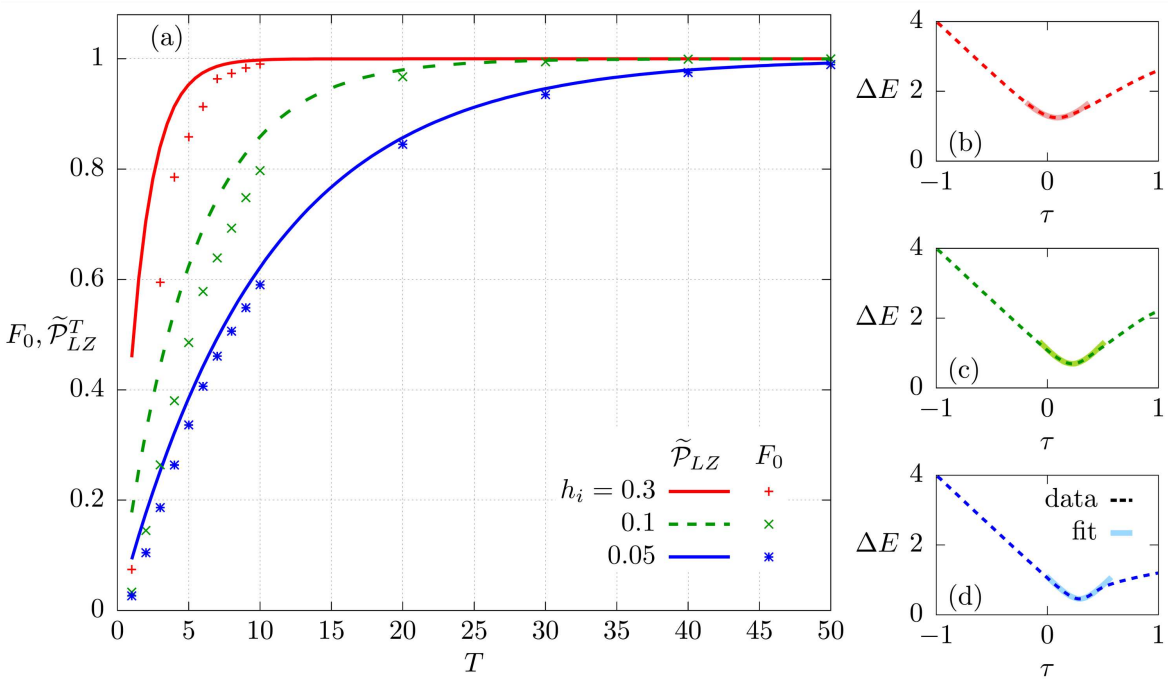

Fig. 3. Comparison of numerical results with the Landau–Zener formula. (a) Numerically obtained projections F_0 (5) for systems with a different uniform h_i (marked with points) and the probability $\widetilde{\mathcal{P}}^T_{\mathrm{LZ}}$ (11) obtained from LZF with a fitted gap (marked with solid or dashed lines) as a function of annealing time T. Blue, green and red colors correspond to different values of fields $h_i = 0.05$, 0.1 and 0.3, respectively. (b)–(d) Numerical results (dashed line) are fitted by (10) (faded bold line). Colors in (a) correspond to colors of dashed lines in panels (b), (c), (d) — for those subfigures $h_i = 0.3$, 0.1 and 0.05, respectively. Results for a chain with open boundary conditions and $L = 12$, $J_{ij} = 1$, $\Delta_i = 2$.

where σ_i^x, σ_i^z are Pauli spin operators, e.g. $\sigma_i^z = 2s_i^z$, J_{ij} denotes interaction between two components of spins on i and j sites, h_i is the value of an external magnetic field (z direction) coupled to spin on site i and Δ_i is the value of a transverse field (x direction). For simplification and without loss of generality, we assume that $A(\tau)$, $B(\tau)$ are linear time-dependent functions which satisfy: $A(-1) = 1$ and $A(1) = 0$, $B(\tau) = 1 - A(\tau)$ and $\tau \in [-1, 1]$. One can notice that in the current D-Wave machines $A(\tau)$, $B(\tau)$ are slightly different [28]. At the end of the evolution, only the second term of (4) remains which is classical. However, in the beginning the evolution starts only with the first term of (4). The initial state is chosen as the ground state for $\hat{H}(-1)$ which may be obtained from the Lanczos algorithm [29–31]. Therefore, (2) is solved for the appropriate time-dependent protocol for functions $A(\tau), B(\tau)$. The evolution of the ground state is obtained by the expansion of a propagator operator in the Chebyshev polynomial basis [32–34] with a sufficiently small time step $\delta t = 0.01$.

4. Results and discussion

The model presented in the previous section is studied for a non-zero value of the external field $h_i \neq 0$. The obtained results are compared with analytic results for a two-level system, i.e., given by the Landau–Zener formula (LZF).

4.1. Comparison of quantum annealing solution to Landau–Zener formula

Here we present the results for other quantities which can be used as an estimation of annealing time T which is sufficient for adiabatic evolution. Instead of calculating kinks in the system or state, and ground state energy difference, one can simply calculate the projection of state to the ground-state $|\langle\psi_0|\psi\rangle|^2$ of the final Hamiltonian [35]. This quantity $|\langle\psi_0|\psi\rangle|^2$ contains information about the probability that a state $|\psi\rangle$, obtained from TDSE, is the ground state $|\psi_0\rangle$ of the final Hamiltonian (4) at $\tau = 1$, obtained from TISE. Figure 3a (with points) shows projection F_0 as a function of T for a system with uniform h_i:

$$F_0 = |\langle\psi_0|\psi\rangle|^2. \tag{5}$$

As it can be seen, even a relatively small value of constant field h_i can rapidly increase the probability of success.

In addition to probability studies, we try to compare our system to the dynamics of a simple two-level system. The latter is described by the time-dependent Hamiltonian [36]

$$\hat{H}_{\mathrm{LZ}}(t) = \frac{1}{2}\alpha t\sigma_z + \frac{1}{2}\beta\sigma_x, \tag{6}$$

where α is the sweeping rate of energy bias and β is the coupling matrix constant.In fact, such a system

can be studied exactly. The transition probability is given by the Landau–Zener formula [37–40]:

$$\mathcal{P}_{\mathrm{LZ}} = \exp\left(-\frac{\pi\beta^2}{2\alpha}\right). \tag{7}$$

However, we are interested in the opposite event. The system should remain in its ground state and then probability should be expressed by:

$$\widetilde{\mathcal{P}}_{\mathrm{LZ}} = 1 - \mathcal{P}_{\mathrm{LZ}} = 1 - \exp\left(-\frac{\pi\beta^2}{2\alpha}\right). \tag{8}$$

The parameters α and β can be obtained by fitting of the energy spectrum. Gap ΔE for LZF can be expressed by subtracting both eigenvalues of the Hamiltonian (6):

$$\Delta E = \sqrt{(\alpha\tau)^2 + \beta^2}. \tag{9}$$

In our case, we use this expression to fit the difference between the two lowest eigenenergies obtained from numerics. Here, the minimum of the gap is not always at $t = 0$ and the gap does not have a symmetric shape. As a result, another parameter τ_0 must be added to the expression for the gap:

$$\Delta E = \sqrt{\alpha^2(\tau - \tau_0)^2 + \beta^2}. \tag{10}$$

Since LZF was derived for an infinite time range $t \in [-\infty, \infty]$, one should introduce the proper scaling of (8) to a finite time range $t \in [-T, T]$ by rescaling $\alpha \to \alpha/T$:

$$\widetilde{\mathcal{P}}^{T}_{\mathrm{LZ}} = 1 - \exp\left(-\frac{\pi\beta^2}{2\alpha}T\right). \tag{11}$$

In Fig. 3b–d gaps for our system are presented. A fitted formula (10) is marked with a faded, bold line. The fitting has to be performed within a limited range of energies, as close as possible to its energy difference minimum because of the lack of symmetry. In Fig. 3a solid/dashed lines show probabilities of remaining in a ground state from the Landau–Zener formula with fitted parameters α, β from the gap. As it can be observed, results from LZF and the actual data differ slightly. Knowing the gap structure, LZF can give an efficient estimation for the proper annealing time T.

5. Summary

We discuss the adiabatic quantum computations, using the Hamiltonian which is relevant for the D-Wave quantum annealers. We compare quantum dynamics obtained from quantum annealing with the approximate expression resulting from the Landau–Zener formula. Simultaneously, we stress the important role of the energy structure during quantum evolution. The bigger the minimum of the energy gap on the entire evolution path, the bigger the probability of observing the system in its ground state. We also check sufficient conditions for the adiabatic evolution. Research on quantum annealers is crucial due to their near-future applications.

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