Staying adiabatic with unknown energy gap

J. Nehrkorn,1 S. Montangero,1 A. Ekert,2,3 A. Smerzi,4 R. Fazio,5 and T. Calarco3

1Institut für Quanteninformationsverarbeitung, Universität Ulm, Albert-Einstein-Allee 11, 89081 Ulm, Germany.
2Mathematical Institute, University of Oxford, 24-29 St. Giles, Oxford, OX1 3LB, United Kingdom.
3Centre for Quantum Technologies, National University of Singapore, 3 Science Drive 2, 117543 Singapore.
4BEC Center, Dipartimento di Fisica Università di Trento, Via Sommarive 14, I-38123 Povo, Italy.
5NEST, Scuola Normale Superiore and Istituto Nanoscienze-CNR, Piazza dei Cavalieri 7, I-56126 Pisa, Italy.

We introduce an algorithm to perform an optimal adiabatic evolution that operates without an apriori knowledge of the system spectrum. By probing the system gap locally, the algorithm maximizes the evolution speed, thus minimizing the total evolution time. We test the algorithm on the Landau-Zener transition and then apply it on the quantum adiabatic computation of 3-SAT: The result is compatible with an exponential speed-up for up to twenty qubits with respect to classical algorithms. We finally study a possible algorithm improvement by combining it with the quantum Zeno effect.

Adiabatic evolution has been used as a standard driving tool for quantum systems evolutions for decades. The Adiabatic Theorem guarantees that a quantum system, prepared in the ground state of a time-dependent Hamiltonian, will stay close to its instantaneous ground state if the Hamiltonian governing the evolution is varied slowly enough, i.e. adiabatically [1]. The most ubiquitous application of this theorem is the solution of quantum mechanical time evolutions in terms of simpler static problems: if the adiabatic condition is fulfilled during the evolution, i.e. the Hamiltonian is varied slowly with respect to the instantaneous energy gap, one knows that the quantum system is described by the instantaneous ground state of the Hamiltonian. A more recent application of the adiabatic theorem has been pointed out to define a new quantum computation model, adiabatic quantum computation (AQC) or quantum annealing [2, 3]. Indeed, if it is possible to define a Hamiltonian whose initial ground state is easy to prepare and whose final ground state encodes the solution to a computational problem, the system can be used as a quantum computer, with the same computational power as the circuit model quantum computation [4]. In the AQC model, the computational complexity is defined via the scaling of the time to reach the final state (containing the solution to the problem), as a function of the size of the input to the problem. Even though, there have been discussions about the consistency of the adiabatic theorem and the sufficiency of its conditions [5, 6], since the introduction of AQC, different interesting applications have been found, like for example the Grover Search problem where the well known quadratic speed-up can be found analytically by locally probing the system adiabaticity [7, 8].

As stated before, the simplest formulation of the adiabatic condition states that the time needed to perform an adiabatic evolution scales as the inverse of the minimal energy gap between the ground and the first excited state [1]. The problem of finding the time-optimal AQC has been put forward recently and reformulated also in geometrical terms [9–11]. However, in all these standard approaches it is necessary to know the instantaneous spectrum of the system under consideration. This task might be very difficult or even impossible, like for example when dealing with quantum systems composed by a large number of particles. Moreover, there are classes of problems, such as the k-SAT studied here, where different instances of different Hamiltonians have to be considered: each of them with a different energy spectrum to be computed. Very recently, Quan and Zurek introduced a method to circumvent this problem by using a quenched echo [10] . The idea is to propagate the ground state of the system forward and backward in time comparing the resulting states to evaluate the adiabaticity of the evolution. Here, we introduce another scheme to find an adiabatic evolution of a given system completely independently of any knowledge of the instantaneous spectrum: we probe locally (in time) the adiabaticity of the system and adjust the local speed to stay close to the instantaneous ground state. We apply this technique to the Landau Zener transition [18] as testbed and then to the computationally hard problem of 3-SAT. Finally, as expected and already shown in a similar setting in [17], we show that combining the algorithm with the quantum
We also used the Quantum Fisher Information (QFI) for as a natural measure of the adiabaticity of the process. Here we choose the energy difference between the result-

function of the errors accumulated during the evolution. Indeed, the overall final excitation of the evolved state is a

time according to a given function $s(t)$ that increases monotonically from $s(0) = 0$ to $s(T) = 1$, where $T$ is the
total evolution time. Our goal is to find the fastest possible way to perform such transformation while still obtaining
an adiabatic transformation within a given error $\epsilon$. To find such evolution, without using any apriori knowledge
of the system spectrum and instantaneous ground state, we evolve the system state $|\Psi(t)\rangle$ by varying the system
parameter from $s(t)$ at time $t$ with velocity $v = \Delta s/\Delta t$, with two different small velocities $v_{\pm} = v(1 \pm \delta)$. In
general, the system ends in two slightly different states that we compare to evaluate the adiabaticity of the evolu-

tion. Indeed, since the energy spectrum is bounded from below, the two states are some excited states above
the ground state. If the two states are almost equal, it means that both velocities $v_{\pm}$ satisfy the adiabaticity condi-
tion and the system is in the instantaneous ground state, that is, we are performing an adiabatic evolution. It is
then possible to increase the velocity $v$ to obtain the fastest possible adiabatic transformation. The limiting
case where the error induced by the transformation with velocity $v_-$ is below the threshold while the other,
induced by $v_+$, is above can be used to determine the maximal velocity allowed for an adiabatic transformation
within a certain tolerance.

The idea presented above can be recast in a simple algorithm as illustrated in Fig. 1:

1. At $t = 0$ prepare the system in the ground state of $\hat{H}(0)$, i.e., $|\Psi(0)\rangle = |\Phi(0)\rangle$.
2. Propagate the system wave function from $|\Psi(t_i)\rangle$ to $|\Psi(\pm)\rangle$, changing $s$ to $s + \Delta s$ with $v_{\pm} = v_i(1 \pm \delta)$ in time $\Delta t = \Delta t/(1 + \delta)$.
3. Evaluate the distance $\epsilon_i$ between $|\Psi(\pm)\rangle$.
4. Maximize $v_i$, such that $\epsilon = \epsilon_{\text{max}}$.
5. Repeat 2 to 4 until $s(t) = s(T) = 1$.

The free parameters $\epsilon_{\text{max}}$ and $\delta$ are the maximum error that we allow per step, and the difference between the
propagating velocities. By choosing $\Delta t$ and $\epsilon_{\text{max}}$ appropriately, it is possible to control the final evolution
time $T$ and thus the final fidelity $F(T) = \left(|\langle \Phi(0) | \Phi(T) \rangle|^2 \right)$. Indeed, the overall final excitation of the evolved state is a function of the errors accumulated during the evolution.

The error or distance per step $\epsilon_i$ between the states $|\Psi(\pm)\rangle$ can be quantified by different figures of merit. Here we choose the energy difference between the result-

ing states

$$\epsilon_1 = \Delta E = \langle \Psi(+) | \hat{H} | \Psi(+) \rangle - \langle \Psi(-) | \hat{H} | \Psi(-) \rangle$$

as a natural measure of the adiabaticity of the process. We also used the Quantum Fisher Information (QFI) for

$$\epsilon_2 = F_Q^+ - F_Q^-$$

where $F_Q = 4(\Delta H)^2 = \langle H^2 \rangle - \langle H \rangle^2$. The QFI can be seen as a statistical distance between quantum states and is a more elaborate method of comparison than the energy difference. However, as we show in the follow-
ing, the final result is not crucially dependent on the choice of the figure of merit. To avoid unphysical “kinks” in the evolution parameter (when the value of the velocity $v$ changes discontinuously from $v_i$ to $v_{i+1}$) that would introduce spurious excitations in the system, we smooth the transition using the error function $v(t) = (v_{i-1} - v_i) \text{erf}[9(t - t_{i-1})/\Delta t] + 1/2(v_i + v_{i-1})$ for $t \in [t_{i-1}, t_i]$.

First of all, as a testbed of the proposed algorithm, we search for the optimal adiabatic Landau-Zener (LZ) transition showing its effectiveness. The adimensional two-level time dependent LZ Hamiltonian is given by

$$H_{LZ} = J = \sigma_x + s(t) \sigma_z$$

where $\sigma_z$ and $\sigma_x$ are the Pauli spin matrices [18] (we set from now on $h = 1$). We control the adiabatic transfor-
mation between the initial and final ground states of the Hamiltonian $|\Phi(0)\rangle$ and $|\Phi(T)\rangle$ by applying the algo-

rithm introduced above. In Fig. 2 we report the final infidelity as a function of the total evolution time $T$ for different values of the time step $\Delta t$ and local error $\epsilon_{\text{max}}$, obtained using both the energy difference and the Fisher information as a local measure of error. As it can be
clearly seen, in a wide range of parameters the data collapse onto two distinct lines (corresponding to the different local error measure $\epsilon$) following the power law

$$1 - F(T) \sim T^{-2} \sim \frac{\epsilon_{\text{max}}}{\Delta t^2}. \quad (4)$$

Fluctuations around this scaling law increase for shorter times, however the agreement is almost perfect on two orders of magnitude in time and on four in the infidelity. As expected, longer times $T$ allows for better fidelities and the total evolution time $T$ is determined by the choice of the algorithm parameters $\epsilon_{\text{max}}$ and $\Delta t$. We stress that the results slightly depend on the error measure $\epsilon_i$ as only the prefactor significantly changes, suggesting that the outcome of the algorithm is independent on the details of the error measure. The important information is whether $|\Psi(\pm)\rangle$ are different, not how this is measured. Similar results have been obtained on different systems, like the adiabatic version of the Grover search algorithm (data not shown). Note that, from the fit of Fig. 2 while using the Fisher information ($\epsilon_{\text{max}} = F_Q^2$), assuming that the Fisher information of the state $|\Psi^-\rangle$ can be neglected, i.e. that the latter is nearer to the ground state), we obtain that the total error is equal to

$$1 - F(T) \simeq \frac{F_Q}{4\Delta t^2}. \quad (5)$$

We can compare Eq. (5) with the standard perturbative expression for the infidelity of a slightly perturbed state $|\Phi\rangle$:

$$1 - F(\tau) = \frac{F_Q \tau^2}{4}, \quad (6)$$

obtaining the relation $\tau = 1/\Delta t$: allowing a maximal error $\epsilon_{\text{max}}$ every time $\Delta t$ results in an overall perturbative process with effective time $\tau$. That is, if $\Delta t \to \infty$ the process is exact.

We then apply the proposed algorithm to an adiabatic quantum computation used to solve a paradigmatic classically hard problem – $k$-SAT – showing how it allows to find a solution with a scaling with the input size that could be exponentially faster than the classical one. Given $n$ Boolean variables, the disjunction of $k$ variables (possibly negated) defines a clause: the conjunction of $m$ clauses is an instance of the $k$-SAT problem. The search for an assignment for all variables such that all clauses of the instance are satisfied at the same time defines the satisfiability problem. The complexity of this problem heavily depends on the ratio of clauses and variables $\alpha = m/n$ and for classical algorithms, the critical value for which the satisfiability problem becomes hard is around $\alpha \simeq 4.3$ [22]. To find the hard instances to test our algorithm, we created sets of thousand instances of 3-SAT for different values of $\alpha$. We then solved them with the classical DPLL algorithm and chose the classically hardest clauses [23]. These clauses showed an exponential increase in the number of iterations of the DPLL-algorithm for $\alpha \sim 4.4$ already with moderate system sizes that can be simulated in the quantum case [23].

The corresponding quantum problem is defined along the lines of [2] and simulated via adiabatic quantum computation using the algorithm presented before. In Fig. 3 we show the scaling of the total running time $\bar{T}$ as a function of the number of qubits. Although the scaling is still not conclusive, the best fit to the data is a sub-exponential fit, namely a quadratic function which is in agreement with the results in [2, 24]. The inset shows the difference between the ten best (ten worst) instances and the mean total running time $\bar{T}$ and the standard deviation $\sigma$ as a function of the number of qubits. Note that the width of the distribution for the total running time appears to reach a constant value as a function of the number of qubits: thus, the scaling of the average running time determines the complexity of the algorithm, giving an indication that no pathological clauses exist.

Finally we investigate the possible combination of the presented algorithm with the Quantum Zeno effect, where a quantum system can be frozen in its state by repeated measurements [19]. It is somehow natural to combine it with our approach, by introducing a periodic measurement of the energy of the system at regular time intervals $t_z$. At each measurement there is a probability $\sigma$ to end in the instantaneous ground state given by $P_z = \langle |\Psi(\Phi^0(t))| \rangle^2$; the overall probability to end in the final ground state is the product $P_{n_z} = \prod_{i=1}^{n_z} P_z$, where $n_z = T/t_z$ is the number of Zeno measurements. As a manifestation of the Quantum Zeno effect, both $P_{n_z}$ and

![FIG. 3: Mean total running time $\bar{T}$ for 100 different instances of 3-SAT as a function of the number of qubits $n = 5, \ldots, 20$ and $\epsilon_{\text{max}} = 3.4 \cdot 10^{-6}$, $\Delta t = 0.1$, $\delta = 0.5$. The fits are a linear (dashed green), quadratic (solid blue) and an exponential function (dashed red). The adjusted coefficient of determination $R^2$ are .98824, .9974 and .9627 for the linear, quadratic and exponential respectively. Inset: Distance of ten best (blue) (ten worst (green)) instances from $\bar{T}$ and distribution standard deviation $\sigma$ (red) for $n = 4, \ldots, 20$.](image-url)
FIG. 4: Upper panel: Final infidelity $1 - F(T)$ as a function of the time between Zeno measurements $t_z/T$ (symbols) normalized to the total time $T$ and without Zeno measurements $n_z = 0$ (lines) for different total time $T = 12.2, \delta t = 0.1$ (green data) and $T = 99.2, \delta t = 0.1$ (blue data) and $\delta t = 0.8$. Lower panel: Final excitation probability $1 - P_{n_z}$ (Probability of algorithm failure) as a function of $t_z/T$ for $T = 12.2$ (green crosses) and $T = 99.2$ (blue circles).

The final fidelity should increase for larger $n_z$ \cite{17}. Moreover, for faster, i.e. less adiabatic evolutions, the effect should be more significant as the projective measurement will ensure that the system remains in the ground state.

In Fig. 4 the infidelity $1 - F(T)$ and probability $1 - P_{n_z}$ to leave the ground state are plotted against the normalized time between Zeno measurement $t_z/T$ for two different total evolution times $T$. The results clearly indicates that the two total times chosen, almost one order of magnitude apart, corresponds to a non-adiabatic and an adiabatic evolution. We normalize the Zeno time $t_z$ to fairly compare such different time scales. The upper panel of Fig. 4 shows that the final infidelity decreases for shorter intervals $t_z/T$, i.e. more measurements, as one would expect. However, when compared with the final infidelity without Zeno measurements (full lines) a big improvement can be seen in the region $0.01 \lesssim t_z/T \lesssim 0.1$ for the non-adiabatic case (more than four orders of magnitude) while in the other case about one order of magnitude can be gained. In the lower panel of Fig. 4, we report the corresponding probability of the algorithm failure $1 - P_{n_z}$ as a function of $t_z/T$. Here, the two different kinds of evolutions studied are clearly visible: in the case of the adiabatic evolution, the probability of exciting the system is greater in presence of the Zeno measurements, while in the non-adiabatic case the Zeno measurements helps the systems to remain in the ground state. Indeed, in the latter case, for $0.01 \sim t_z/T$ there is an improvement of the final fidelity of about four orders of magnitude with a chance of failure of only a few percent: for very fast evolutions exploiting Zeno effect is a successful strategy to improve the algorithm convergence.

In conclusion, we introduced an algorithm to optimize an adiabatic transition for an arbitrary time dependent quantum system with total ignorance of the instantaneous eigenstates and the resulting gap of the system. Numerical simulations showed an expected correlation between the total running time and the final fidelity which does not largely depend on the comparison method used for the evaluation of the adiabaticity of the evolution of each step. We applied the algorithm to the 3-SAT problem and reproduced the results obtained by \cite{2}, suggesting an exponential speed-up of the adiabatic computation with respect to the classical one. Finally, we combined the algorithm with the quantum Zeno effect to further improved the results for very fast (non-adiabatic) transitions. As a final note, we mention that the algorithm effectively measures the size of the instantaneous gap, thus it can be used to investigate systems with a closing gap, also in combination with numerical techniques such as tensor network methods where the full knowledge of the system spectrum is out the computational capability of actual classical computers.

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