Speed limits for quantum gates in multi-qubit systems

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We use analytical and numerical calculations in order to obtain speed limits for various unitary quantum operations in multi-qubit systems. The operations that we consider include single-, two- and three-qubit gates, as well as quantum state transfer in a chain of qubits. We find in particular that simple methods for implementing two-qubit gates generally provide the fastest possible implementations of these gates. We also find that the three-qubit Toffoli gate time varies greatly depending on the type of interactions and the system’s geometry, taking only slightly longer than a two-qubit CNOT gate for a triangle geometry. The speed limit for quantum state transfer across a qubit chain is set by the maximum spin wave speed in the chain.

I. INTRODUCTION

There are a number of candidate physical systems for the implementation of qubits in a future quantum computer [1]. Single-, two- and three-qubit gates have been implemented in some of these systems in the past few years. Various other quantum-information-related tasks based on collective manipulation of qubits have also been demonstrated on larger systems [1].

As qubit systems advance towards large-scale demonstrations and practical applications, it becomes increasingly important to optimize the time required to implement the different operations, such that the maximum number of operations is achieved within the coherence time of the system. This goal is the main motivation of this work.

The question of time-optimal control has already been discussed in a number of studies in the literature. For example, Refs. [2, 3] considered optimized constructions of general quantum gates using sequences of basic gates. References [4] discussed the relationship between speed limits on quantum gates and the different energy scales in a physical system, while Refs. [5] explored the analogy between the problem of finding the minimum times for quantum gates and the problem of finding geodesics in curved spaces. The time-optimal implementation of the Quantum Fourier Transform in multi-qubit systems was analyzed in Ref. [6]. References [4, 10] performed numerical calculations in order to determine the minimum time required for quantum gates in specific experimental setups based on superconducting qubits. The speed limit on quantum state transfer in long spin chains has also been studied recently [7, 8].

Here we consider a number of important operations in a variety of possible setups, with varying degrees of single-qubit control and inter-qubit coupling mechanisms. We use analytical control and numerical calculations based on optimal control theory in order to give speed limits for these operations.

The paper is organized as follows: In Sec. I we introduce the different possible setups, with varying forms of single-qubit controls and interactions. We then discuss the speed limits of single-qubit gates (Sec. II), two-qubit gates (Sec. III) and three-qubit gates (Sec. IV). In Sec. V we discuss the problem of quantum state transfer. We conclude with a brief summary of the results in Sec. VII.

II. DIFFERENT TYPES OF QUBITS AND THEIR COUPLING

Over the years, various physical systems and designs have been proposed and demonstrated as implementations of qubits. This variety means that the degree of control in qubit manipulation and the physical mechanisms for coupling between qubits vary from one system to another. In some cases, the qubit is formed by the lowest two energy levels of a multi-level quantum system, adding complications to the control requirements of the qubit. Here we shall focus on “good” qubits, where a description with only two quantum states provides a good approximation of the physical system.

With the assumption of two-state qubits, the single-qubit Hamiltonian can be expressed in terms of the two-dimensional Pauli matrices $\sigma_\alpha$ (with $\alpha = x, y$ or $z$):

$$\hat{H} = -\frac{\Delta(t)}{2}\hat{\sigma}_x - \frac{\epsilon(t)}{2}\hat{\sigma}_z,$$

(1)

where the time dependence in Eq. (1) suggests that both $\Delta$ and $\epsilon$ are tunable. Some experimental setups (e.g. early experiments on superconducting qubits) have only one tunable parameter, typically expressed as $\epsilon$ in Eq. (1). We shall consider both cases below.

Driving signals used for the manipulation of the qubits can be applied through the tunable parameters in the Hamiltonian. We shall assume that any arbitrary driving signal can be applied to the system. In other words, we look for the fastest implementation of quantum operations in the space of all possible control signals.
The coupling Hamiltonian between two qubits is typically of Ising or Heisenberg form. The former is described by the Hamiltonian

$$\hat{H}_I = J \hat{\sigma}_z^{(i)} \otimes \hat{\sigma}_z^{(j)},$$  \hspace{1cm} (2)

while the latter is described by the Hamiltonian

$$\hat{H}_H = J \left( \hat{\sigma}_x^{(i)} \otimes \hat{\sigma}_x^{(j)} + \hat{\sigma}_y^{(i)} \otimes \hat{\sigma}_y^{(j)} + \hat{\sigma}_z^{(i)} \otimes \hat{\sigma}_z^{(j)} \right).$$  \hspace{1cm} (3)

where $J$ is the coupling strength and the superscripts $i$ and $j$ denote the two coupled qubits. There are situations where the coupling strength is tunable, e.g. using additional coupler elements in the system. However, since we are interested in the speed limits for performing multi-qubit gates, we shall assume that one would want to set $J$ at its maximum achievable value and therefore treat $J$ as a fixed parameter in the calculations below. It is worth mentioning here that it is possible in principle to have fixed values of $\Delta$ and $\epsilon$ and still be able to obtain the desired gates via the modulation of $J$, an approach sometimes referred to as parametric coupling [11].

The parameters of the single-qubit Hamiltonian are typically much larger than the inter-qubit coupling strength, i.e. $J \ll \Delta, \epsilon$. This separation in energy scales simplifies the process of identifying the central elements in the speed limits found in our calculations, and it makes the results easily applicable to different setups.

III. SINGLE-QUBIT GATES

Since the parameters of the single-qubit Hamiltonian are typically much larger than the inter-qubit coupling strength, one can ignore inter-qubit interactions when performing single-qubit gates. Furthermore, performing single-qubit gates typically takes a negligibly short duration compared to the duration required for performing a two- or multi-qubit gate, such that the time required for performing single-qubit gates is usually ignored for purposes of evaluating the computational cost of a given multi-qubit task.

Ignoring interactions, and thus reducing the problem of finding optimal pulses and speed limits for performing a given single-qubit gate to a single-qubit problem, the task at hand becomes straightforward. A common situation is that where one of the two parameters, say $\epsilon$, is tunable over a much larger range than the other one, while the other parameter is either fixed or tunable over a much smaller range. A rotation by an angle $\beta$ about an axis that makes an angle $\theta$ with the $xz$-axis and an angle $\phi$ with the $xz$ plane can be implemented as follows: rotate the state by an angle $-\phi$ about the $z$-axis, set the Hamiltonian to $-\Delta(\hat{\sigma}_z - \hat{\sigma}_z / \tan \theta)/2$ and let it act for a duration $\beta \cos \theta/\Delta$, and finally rotate the state by an angle $\phi$ about the $z$-axis. The first and last steps are fast operations, leaving the duration of the second step as the minimum time required for implementing the desired rotation. One can therefore say that the speed limit is set by the smaller of the two qubit parameters (or more accurately the smaller of the largest achievable values of the two parameters), which in the above example is $\Delta$.

IV. TWO-QUBIT GATES

We start the discussion of finding the speed limits for two-qubit gates by mentioning two approaches that might seem promising at first sight, but to our knowledge are not easily applicable to the problem at hand. First, there are expressions for the speed limits of quantum operations based on the energy and the spread in energy of the quantum state [4]. The reason why these arguments do not apply straightforwardly here can be seen by considering two qubits with a coupling strength that is much smaller than the inter-qubit detuning. The energy scales of the combined system are then, to a very good approximation, set by the individual qubit energies and their detuning from each other. The coupling strength only slightly modifies the energy eigenstates and eigenvalues. The coupling strength must, however, be the limiting factor for performing two-qubit gates. The larger energy scales can probably be used to set a lower bound on the required gate time (i.e. an upper bound on the speed). However, the coupling strength would give a much higher lower bound.

The other approach is that where two-qubit gates are visualized using geometric representations, and the process of performing a two-qubit gate is seen as the motion of the system’s propagator through the space of all two-qubit quantum operations [5]. This approach does indeed provide an intuitive view of the problem and can be very useful in calculations. However, to our knowledge it is only in special cases that this approach can be used to provide an analytical expression for the speed limit for a given two-qubit gate and a given form of inter-qubit interaction.

Here we use numerical calculations in order to find the speed limits for a number of standard two-qubit gates. The method is based on optimal control theory for finding driving pulses that maximize the gate fidelity [12] (The fidelity is essentially a measure of the overlap between the numerically calculated gate and the desired gate). When the gate time (which is a variable parameter in the calculations) is set to a small value, the maximum achievable fidelity is substantially smaller than unity. As the allowed time is increased, the maximum achievable fidelity increases, until at a certain value of the allowed time the fidelity reaches the value one and remains at that value for larger times [6, 8]. In other words, when plotted as a function of the allowed time, the fidelity exhibits non-analytic behaviour as it suddenly hits the value one and remains there. The time at which the fidelity reaches unity defines the minimum gate time, which can alternatively be expressed as the speed limit. A commonly used procedure for deducing speed limits is to set a threshold value for the fidelity (say 99%) and numerically identify
the minimum time required in order to attain this fidelity. This procedure is illustrated in Fig. [1]

Here we use an alternative procedure that avoids one of the drawbacks of the above procedure, namely the slow convergence of the pulse-optimization algorithm when the fidelity approaches unity. We calculate the maximum achievable fidelity for times varying between zero and an estimated value for the minimum gate time. The results of such a calculation are plotted in Fig. [4] for the case of the $\sqrt{\text{SWAP}}$ gate with Heisenberg interactions. We can see that the results fit very well with a function that gives the expression $\pi/(8J)$ for the minimum gate time [It will be explained shortly why this expression is to be expected]. The sine function used in the figure was used as a ‘trial’ fitting function; it was inspired by the behaviour of single-qubit gates but turned out to produce an excellent fit in this case as well. We note here that this alternative method (i.e. the method where one looks away from the threshold region in order to identify the minimum gate time) has not been used in the literature in the context of optimal-control theory. More complicated fitting functions might be required when applying this method to systems with more than two qubits. However, it would be interesting to explore in the future the usefulness of this approach to similar problems. We shall use this method when identifying the minimum gate time in the calculations below.

The gates that we consider here are: iSWAP, CZ, CNOT and $\sqrt{\text{SWAP}}$. There are a number of simple methods that can be obtained using intuition for the implementation of these gates assuming a given (fixed) coupling strength $J$ and tunable single-qubit parameters. The basic techniques are summarized in the following [13]:

**iSWAP Gate:** The standard approach to implementing the iSWAP gate with Ising interactions is to put the two qubits in resonance with each other, i.e. setting $\Delta_1 = \Delta_2 = \Delta$, with $\epsilon_1 = \epsilon_2 = 0$ and $J \ll \Delta$:

\[
\hat{H} = -\frac{\Delta_1}{2} \sigma_x^{(1)} - \frac{\Delta_2}{2} \sigma_x^{(2)} + J \sigma_z^{(1)} \otimes \sigma_z^{(2)} \\
\approx -\frac{\Delta}{2} \sigma_x^{(1)} - \frac{\Delta}{2} \sigma_x^{(2)} + J \left( \sigma_+^{(1)} \otimes \sigma_-^{(2)} + \sigma_-^{(1)} \otimes \sigma_+^{(2)} \right)
\]

(4)

where the operators $\sigma_{\pm}$ are raising and lowering operators that excite or de-excite the individual qubits between their single-qubit energy eigenstates, which in this case are the eigenstates of $\sigma_x$. When allowed to act for a duration $t = \pi/(2J)$, the Hamiltonian in Eq. (4) effects an iSWAP gate, in addition to two single-qubit rotations.

**Controlled-$\pi$-Phase gate:** With Ising interactions, the controlled-$\pi$-Phase (or CZ) gate can be performed by setting $\Delta_1 = \Delta_2 = 0$:

\[
\hat{H} = -\frac{\epsilon_1}{2} \sigma_z^{(1)} - \frac{\epsilon_2}{2} \sigma_z^{(2)} + J \sigma_z^{(1)} \otimes \sigma_z^{(2)},
\]

(5)

with no conditions on $\epsilon_1$ and $\epsilon_2$. When allowed to act for a duration $t = \pi/(4J)$, the Hamiltonian in Eq. (5) effects a CZ gate, in addition to two single-qubit rotations and an (unimportant) overall phase factor.

**CNOT gate:** The CNOT gate can be obtained by combining the CZ gate with two single-qubit gates. These are $\pi/2$ pulses applied to the target qubit before and after the CZ gate. As a result, the amount of time required to obtain the CNOT gate using this approach is approximately equal to the amount of time required for the CZ gate, i.e. $\pi/(4J)$ with Ising interactions.

**$\sqrt{\text{SWAP}}$ gate:** The $\sqrt{\text{SWAP}}$ gate is more naturally obtained with Heisenberg interactions. In this case, one sets $\Delta_1 = \Delta_2$ and $\epsilon_1 = \epsilon_2$, and after a time $t = \pi/(8J)$ one obtains the $\sqrt{\text{SWAP}}$ gate.

**Numerical results:** We have performed numerical calculations using the GRAPE algorithm [12] in order to determine the shortest time required for performing each one of the gates mentioned above. The results for the deduced gate times are summarized in Table I. The numerical calculations are performed with 500 time steps and $10^4$ iterations. With these parameters a single data point takes a calculation time on the order of one hour. For fixed-$\Delta$ calculations, we set $\Delta_2/\Delta_1 = 0.9$ and $J/\Delta_1 = 0.01$. All the results remained unchanged whether the parameters $\Delta_i$ were taken to be fixed or tunable.

![FIG. 1: (Color online) The fidelity of the CNOT gate for the pulse obtained using optimal control theory as a function of the allowed time $t$ (plotted in the combination $4Jt/\pi$) in the case of Ising interactions and a fixed gap. The parameters are $\Delta_2/\Delta_1 = 0.9$ and $J/\Delta_1 = 0.01$. The dashed line represents a possible threshold fidelity for identifying the minimum gate time. Here this threshold is set at 0.98.](image-url)

**V. THREE-QUBIT GATES**

The most well-known three-qubit gate is the Toffoli gate. This gate is also known as the controlled-controlled-NOT gate, because it applies the NOT operation to the target qubit when both control qubits are in the state $|1\rangle$. It has been known for some time that the
TABLE I: Minimum times required for various two-qubit gates and physical realizations. The analytical expressions given below are extracted from the numerical calculations: for each calculation we identify the value of the time that gives a good fit to a figure similar to Fig. 2 (We always obtained good fits).

| Gate          | CNOT          | CZ            | iSWAP         | $\sqrt{\text{SWAP}}$ |
|---------------|---------------|---------------|---------------|-----------------------|
| Matrix        | $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & i & 0 \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1+\frac{i}{2} & 1+\frac{i}{2} & 0 \\ 0 & 1+\frac{i}{2} & 1+\frac{i}{2} & 0 \end{pmatrix}$ |
| Ising         | $\frac{\pi}{4J}$ | $\frac{\pi}{4J}$ | $\frac{\pi}{2J}$ | $\frac{3\pi}{8J}$ |
| Heisenberg    | $\frac{\pi}{4J}$ | $\frac{\pi}{4J}$ | $\frac{\pi}{2J}$ | $\frac{\pi}{8J}$ |

FIG. 2: (Color online) The fidelity of the $\sqrt{\text{SWAP}}$ gate for the pulse obtained using optimal control theory as a function of the allowed time $t$ (plotted in the combination $8Jt/\pi$) in the case of Heisenberg interactions and a fixed gap. The parameters are $\Delta_2/\Delta_1 = 0.9$ and $J/\Delta_1 = 0.01$. The dashed line represents, as an example, a threshold fidelity of 0.98. The red dotted line is the function $(5/8) + (3/8) \times \sin(4Jt)$. Note that the value 5/8 is the fidelity of the unit matrix with the target gate.

Toffoli gate can be constructed from six CNOT gates, in addition to a number of single-qubit gates. Recently it has been shown that this number (i.e. six) is the minimum number of CNOT gates required in order to construct the Toffoli gate [14]. Different constructions based on general conditional gates have also been proposed, reducing the Toffoli-gate time from six to 3.5 times that CNOT gate time [2]. An optimal-control-theory-related calculation based on certain forms of pulses has found a gate time of about 2.2 times the CNOT gate time for qubits coupled in a triangle geometry [3].

We have performed numerical calculations in order to determine the minimum time required in order to obtain the Toffoli gate for a Hamiltonian with pairwise interaction terms given by Eq. (2) or Eq. (3). We should stress here that these calculations are independent of the results mentioned above. The reason is that the gate-counting calculations assume that the different gates are applied as separate, well-defined units, and in some calculations it is assumed that the only two-qubit gate used in the construction are taken from a specific class of gates (e.g. conditional gates). One can therefore expect that it should be possible to obtain a shorter minimum time for the Toffoli gate by considering essentially all the possible driving pulses.

The results are summarized in Table II. There we show results where all coupling strengths are equal (Allowing small differences between the different coupling strengths does not change the main results). We only present results for fixed-$\Delta$ calculations, because the variable-$\Delta$ calculations did not produce any useful results within any reasonable calculation time. In addition to the fact that our procedure typically overestimate the minimum gate time, we would like to point out the the results presented in Table II also showed relatively strong dependence on the guess pulses. In response to this observation, we have used a number of different patterns for the guess pulses. We cannot however, exclude the possibility that some of the expressions in the table are substantially larger than the true minimum gate time. For the triangle geometry, we find Toffoli gate times that are smaller than twice the minimum time required for a CNOT gate with the same coupling strength. In this case, we can have a good level of confidence that the results are at least close to the true minimum gate time, since it seems implausible that the Toffoli gate could be faster than the CNOT gate for the same value of the coupling strengths. From the results shown in the table, we can also conclude that having the qubits connected in a triangle geometry would be desirable for purposes of implementing fast three-qubit gates. We should point out here that these results give faster gates than any results for the maximum speed of Toffoli gates in the literature [2, 3]. In particular, one can compare the factor 1.6 in Table II with the corresponding factor of 2.2 in Ref. [3]: an improvement of about 27%.
VI. QUANTUM STATE TRANSFER IN A CHAIN OF QUBITS

Another operation in multi-qubit systems that has received considerable attention in recent years is that of quantum state transfer across a chain of qubits [15]. In this section we provide analytical expressions for the speed limit of state transfer across a long chain.

The Hamiltonian for a qubit chain with nearest neighbour interactions is given by

$$\hat{H} = \sum_{i=1}^{N} \left( -\frac{\Delta_i}{2} \hat{\sigma}_z^{(i)} - \frac{\epsilon_i}{2} \hat{\sigma}_z^{(i)} \right) + \sum_{i=1}^{N-1} J_i \hat{\sigma}_z^{(i)} \otimes \hat{\sigma}_z^{(i+1)}$$

(6)

for the case of Ising interactions and

$$\hat{H} = \sum_{i=1}^{N} \left( -\frac{\Delta_i}{2} \hat{\sigma}_z^{(i)} - \frac{\epsilon_i}{2} \hat{\sigma}_z^{(i)} \right) + \sum_{i=1}^{N-1} J_i \times$$

$$\left( \hat{\sigma}_x^{(i)} \otimes \hat{\sigma}_x^{(i+1)} + \hat{\sigma}_y^{(i)} \otimes \hat{\sigma}_y^{(i+1)} + \hat{\sigma}_z^{(i)} \otimes \hat{\sigma}_z^{(i+1)} \right)$$

(7)

for Heisenberg interactions. The case with fixed and generally disordered values of $\Delta_i$ and/or $J_i$ leads to serious complications (such as Anderson localization), and we therefore do not consider this case. For the case of fixed, uniform values of $\Delta_i$ and $J_i$ or the case of tunable $\Delta_i$ and uniform $J_i$, we can use arguments from band theory to find the speed limit for state transfer.

The state transfer process can be thought of as the process of wave propagation through the chain, as discussed in Ref. [8]. The speed limit is then determined by the maximum group velocity of a wave packet traveling through the chain. We also observe here that wave propagation cannot be sped up through the application of nonuniform external fields. We can therefore calculate the maximum wave speed assuming a uniform external field (i.e. time- and position-independent values of $\Delta_i$ and $\epsilon_i$). For the case of Ising interactions, we start by noting that if we take $\Delta = 0$, the operator $\hat{\sigma}_z^{(i)}$ commutes with the Hamiltonian, prohibiting “propagation”. We therefore conclude that the condition $\Delta \gg J$ is optimal for maximizing the propagation speed. With this assumption, the wave function that describes a wave with momentum $k$ (with $-\pi < k < \pi$) is given by

$$|k\rangle = \sum_{j=1}^{N} e^{ijk} \hat{\sigma}_z^{(j)} |\sigma_z^{(1)} = 1, \ldots, \sigma_z^{(N)} = 1\rangle.$$  

(8)

The energy spectrum of these waves is given by $E_k = 2J \cos k$. The group velocity of the wave is given by

$$v_k = \frac{dE}{dk} = -2J \sin k,$$

(9)

which has a maximum at $k = \pi/2$, and the maximum is given by $2J$. The minimum time for the wave to traverse a chain of length $N$ is attained when the wave is initialized and set to travel at this maximum wave speed. Ignoring chain-length-independent contributions at the beginning and end of the transfer process, the minimum transfer time is therefore given by

$$T_{\text{min}} = N/(2J).$$

(10)

It is worth noting that $T_{\text{min}}$ is faster by a factor of $\pi$ than the sequential application of iSWAP operations across the chain.

For the case of Heisenberg interactions, the speed of wave propagation is independent of the external fields. Taking $\Delta \gg J$, $\epsilon = 0$, and assuming only one excitation in the system, the problem reduces to that with Ising interactions but with twice the coupling strength: the $\hat{\sigma}_z^{(i)} \otimes \hat{\sigma}_z^{(j)}$ term has no effect on the dynamics, and

$$\hat{\sigma}_y^{(i)} \otimes \hat{\sigma}_y^{(j)} + \hat{\sigma}_z^{(i)} \otimes \hat{\sigma}_z^{(j)} = 2 \left( \hat{\sigma}_+^{(i)} \otimes \hat{\sigma}_-^{(j)} + \hat{\sigma}_-^{(i)} \otimes \hat{\sigma}_+^{(j)} \right).$$

(11)

The minimum transfer time is therefore given by

$$T_{\text{min}} = N/(4J).$$

(12)

Using numerical calculations Ref. [8] found a time that is a few percent higher than that given above (note that there is a factor of 2 difference between Eq. (7) and the Hamiltonian used in Ref. [8]).

Even though the maximum wave speed sets an upper limit to the speed of quantum state transfer, one still needs to make sure that the quantum state is transferred without distortion. The authors of Ref. [7] assumed that one has access to a limited number of qubits in the chain and analyzed the dispersion of the propagating wave. They found that if one has access to a number that is at least on the order of $\sqrt{N}$ at both ends of the chain, state transfer can occur with high fidelity. The authors of Ref. [8] assumed access to all the qubits and, using numerical calculations, demonstrated that using a ‘carrier’ external field (i.e., a harmonic-oscillator potential that moves along the chain and carries the quantum state as it moves along) the dispersion of the wave can also be prevented, and high-fidelity state transfer is possible.
VII. CONCLUSION

We have derived a number of speed limits, or lower bounds on the required time, for various quantum operations. Single-qubit operation speeds are limited by the smaller of the Pauli-matrix coefficients in the Hamiltonian. We have used optimal control theory to obtain speed limits for a few well-known two-qubit gates and the three-qubit Toffoli gate. As expected, two-qubit gate speeds are limited by the inter-qubit coupling strength. The Toffoli gate requires approximately two or three times the minimum time required for a CNOT gate in a chain geometry, depending on the form of the interaction term, and less than twice the minimum time required for a CNOT gate in a triangle geometry. Finally, we have used arguments from condensed-matter physics to derive the speed limit for quantum state transfer in a qubit chain. The expressions that we find agrees with recent numerical results.

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