Programming Physical Realizations of Quantum Computers

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We study effects of the physical realization of quantum computers on their logical operation. Through simulation of physical models of quantum computer hardware, we analyze the difficulties that are encountered in programming physical realizations of quantum computers. Examples of logically identical implementations of the controlled-NOT operation and Grover’s database search algorithm are used to demonstrate that the results of a quantum computation are unstable with respect to the physical realization of the quantum computer. We discuss the origin of these instabilities and discuss possibilities to overcome this, for practical purposes, fundamental limitation of quantum computers.

PACS numbers: 03.67.Lx, 05.30.-d, 89.80.+h, 02.70Lq

I. INTRODUCTION

Recent theoretical work has shown that a Quantum Computer (QC) has the potential of solving certain computationally hard problems such as factoring integers \(^1\) and searching databases much faster than a conventional computer \(^2\). In most theoretical work the operation of a QC is described in terms of highly idealized transformations on the qubits \(^3\). The impact of the physical implementation of a QC on its computational efficiency is largely unexplored.

The logical operation of conventional digital circuits does not depend on their hardware implementation (e.g. semiconductors, relays, vacuum tubes, etc.). Dissipative processes suppress the effects of the internal, non-ideal (chaotic) dynamics and drive the circuits into regions of stable operation. Conventional digital computers, built from these digital circuits, are in one particular state at a time and are able to perform logical operations that do not depend on their hardware implementation. From the point of view of programming the computer this is very important. Implementations of algorithms designed to run on a conventional computer will give results that do not depend on the hardware used to build the computer.

A QC differs from a conventional digital computer in many respects. A QC exploits the fact that a quantum system can be in a superposition of states. Interference of these states allows exponentially many computations to be done in parallel \(^3\). The presence of the superposition of states is a direct manifestation of the internal quantum dynamics of the elementary units of the QC, the qubits. In an ideal QC the qubits are assumed to be ideal two-state quantum systems. Therefore, the operation of an ideal QC does not depend on the intrinsic dynamics of its qubits.

A physically realizable QC is a many-body system in which the quantum dynamics of the qubits is essential to its operation. Manipulation of one qubit may cause unwanted motion of other qubits. It is difficult to suppress these effects by dissipation because in contrast to the case of conventional digital circuits, dissipation processes have a devastating effect on the coherent quantum dynamical motion of the qubits. Therefore a quantum algorithm (QA) may yield quantum computation results that depend on the specific physical realization of the QC. Although QA’s can be designed independent of the QC hardware, the implementation of a QA on a physical realization of a QC (i.e. the programming of the QC) very much depends on the hardware of which the QC is built from. We refer to the difficulty of programming QC’s as the Quantum Programming Problem (QPP).

Due to the QPP it may be very difficult to develop a non-trivial quantum program for a physical realization of a QC. Moreover, there is no guarantee that an implementation of a QA, that works well on one QC will also perform well on other physical realization’s of QC’s. As mentioned above, there are several factors that contribute to the QPP:
1) Differences between the theoretically perfect and physically realizable one- and two-qubit operations; qubits cannot be kept still during the time that other qubits are being addressed; precision needed to implement operations on the qubits.

2) The effect of coupling of the qubits to other degrees of freedom (dissipation, decoherence).

In most theoretical work on QC’s and QA’s one considers theoretically ideal (but physically unrealizable) QC’s. Then the QPP is not an issue. The QPP is also fundamentally different from the error propagation previously studied in QA’s implemented on ideal QC’s since the QPP is due to the specific realization of the QC and leads to systematic instead of random errors.

How does a QPP reveal itself? Consider two logically independent operations (O₁ and O₂) of the machine. On a conventional computer or ideal QC, the order in which we execute these two mutually independent instructions does not matter: \( O₁O₂ = O₂O₁ \). However, on a physically realizable QC sometimes the order does matter, even if there are no logical dependencies in these two program steps. In some cases, due to practical problems in manipulating individual qubits \( O₁O₂ \neq O₂O₁ \) and the QC may give wrong answers. Note the qualifier sometimes. There seems to be no general rule to decide beforehand which operation and at what stage of the QA the QPP leads to incorrect results. At present the only way to find out seems to be to actually carry out the calculations and check the results.

In this paper we study the relation between the physical realization of QC’s and their logical operation. We investigate various aspects of the QPP by simulating QC hardware. In this work we only consider effects of the intrinsic quantum dynamics of the QC (item 1, see above). The study of the effect of the coupling of the qubits to other degrees of freedom (item 2, see above) is left for future research. We demonstrate that the programming of a physical, non-ideal implementation of a QC is difficult, even if the QC consists of only two qubits. Berman et al. investigated the influence of the Ising spin interaction on the quantum dynamics of NMR systems. Although they did not address the QPP, the work is similar in spirit to and the present paper as it explores the consequences of the difference between the ideal QC’s and physical realizations of QC’s. For the physical systems and time-scales considered in this paper, the effects of the interactions between the spins are negligible. As far as we know no experimental data has been published that specifically addresses this, for potential applications, very important and intrinsic problem of programming QC’s. However, with the QC hardware currently available a test of correct quantum computation on a physical realization of a QC is definitely within reach. In this paper we propose two simple QA’s that may be used to study the QPP in physical realizations of QC’s. We also discuss methods to enlarge the region(s) of reliable operation.

The paper is organized as follows: In Section II we describe a physical model of a QC. Our choice is largely inspired by NMR-QC experiments, mainly because other candidate technologies for building QC’s are not yet developed to the point that they can execute computationally non-trivial QA’s. As the basic example of a QA we take the Controlled-NOT (CNOT) gate. In Section III we discuss the implementation of the CNOT gate on an ideal two-qubit QC and describe simple, non-trivial QA’s that consist of repetitions of CNOT operations. As an illustration of the general nature of the QPP, we also consider a more complicated example, namely Grover’s QA to search for an item in a database. In Section IV we derive the conditions for which the physical two-qubit QC will exhibit ideal QC behavior and discuss the generalization of these ideas to n-qubit QC’s. Also in Section IV we describe the implementation of the QA’s discussed in Section III on a physical realization of a QC. In Section V we demonstrate and analyze the QPP by simulating the time-evolution of (= execute QA’s on) the physical model of the QC by solving the time-dependent Schrödinger equation. In Section VI we summarize our findings.

II. PHYSICAL MODEL OF A QUANTUM COMPUTER

Generic QC hardware can be modeled in terms of quantum spins (qubits) that evolve in time according to the time-dependent Schrödinger equation (TDSE)

\[
\frac{\partial}{\partial t} |\Phi(t)\rangle = H(t)|\Phi(t)\rangle, \tag{1}
\]

in units such that \( \hbar = 1 \). For present purposes it is sufficient to consider two-qubit QC’s only. The state

\[
|\Phi(t)\rangle = a(\downarrow,\downarrow; t) |\downarrow,\downarrow\rangle + a(\uparrow,\downarrow; t) |\uparrow,\downarrow\rangle + a(\downarrow,\uparrow; t) |\downarrow,\uparrow\rangle + a(\uparrow,\uparrow; t) |\uparrow,\uparrow\rangle, \tag{2}
\]

describes the state of the QC at time \( t \). The complex coefficients \( a(\downarrow,\downarrow; t), \ldots, a(\uparrow,\uparrow; t) \) completely specify the state of the quantum system. In the absence of interactions with other degrees of freedom this spin-1/2 system can be modeled by the time-dependent Hamiltonian.
where \( S^\alpha_j, \alpha = x, y, z \) denotes the \( \alpha \)-th component of the spin-1/2 operator representing the \( j \)-th qubit, \( J \) determines the strength of the interaction between the two qubits, \( h^x_j \) and \( h^y_j \) represent the strength of the applied static (magnetic) and applied sinusoidal field (SF) acting on the \( j \)-th spin respectively. For a physical system, \( h^x_j = \gamma h^x_j \) and \( h^y_j = \gamma h^y_j \), for \( \alpha = x, y, z \) where \( \gamma \) is a constant. The frequency and the phase of the SF are denoted by \( \omega \) and \( \phi_0 \). As the Ising model, i.e. the first term of (3), is known to be a universal QC \([36,37]\), model (3) is sufficiently general to serve as a physical model for a generic QC at zero temperature. In terms of spin matrices, the operator \( Q_j \) measuring the state of qubit \( j \) is given by

\[
Q_j = \frac{1}{2} - S^z_j. \tag{4}
\]

For numerical purposes it is necessary to fix as many model parameters as possible. We have chosen to simulate the two nuclear spins of the \(^1\text{H}\) and \(^{13}\text{C}\) atoms in a carbon-13 labeled chloroform, a molecule that has been used in NMR-QC experiments \([13,14]\). In these experiments \( h^x_2/2\pi \approx 500\text{MHz}, h^y_2/2\pi \approx 125\text{MHz}, \) and \( J/2\pi \approx -215\text{Hz} \) \([16]\). In the following we will use model parameters rescaled with respect to \( h^x_2/2\pi \), i.e. we put

\[
J = -0.43 \times 10^{-6}, \quad h^x_1 = 1, \quad h^x_2 = 0.25. \tag{5}
\]

Note that there is a difference of many orders of magnitude between the interaction \( J \) and the fields \( h^x_j \). If the duration of the SF-pulses is much shorter than \( 2\pi/|J| \), the effects of \( J \) on the time evolution during these pulses are very small. Our numerical experiments (see below) are all performed under this condition. We will only consider QC’s at zero temperature without coupling to the environment. In this sense we simulate highly idealized NMR experiments on a closed quantum system at zero temperature. This allows us to study a concrete physical realization of a QC and at the same time focus on the intrinsic quantum dynamics of the QC.

A QA for QC model (3) consists of a sequence of elementary operations (EO) that change the state \( |\Psi\rangle \) of the quantum processor according to the TDSE, i.e. by (a product of) unitary transformations. Each EO transforms the input state \( |\Psi(t)\rangle \) into the output state \( |\Psi(t + \tau)\rangle \) where \( \tau \) denotes the execution time of the EO. The action of an EO on the state \( |\Psi\rangle \) of the quantum processor is defined by specifying how long it acts (i.e. the time interval \( \tau \) during which it is active), and the values of \( J \) and all \( h^\alpha \)’s. During the execution of an EO the values of \( J \) and all \( h^\alpha \)’s are kept fixed.

The time evolution of quantum model (3) is obtained by solving TDSE (1) for model (3). The simulations have been carried out with a software tool called Quantum Computer Emulator (QCE) \([38]\). The QCE software simulates physical models of QC hardware by a Suzuki product-formula \([33,40]\), i.e. in terms of elementary unitary operations \([11,13]\). For all practical purposes, the numerical results obtained by this technique are exact. A detailed description of the QCE software tool can be found elsewhere \([12]\).

III. IDEAL QUANTUM COMPUTER

A. Single-qubit operations

One qubit or one spin-1/2 system is a two-state quantum system. The two basis states spanning the Hilbert space are denoted by \( |\uparrow\rangle \equiv |0\rangle \) and \( |\downarrow\rangle \equiv |1\rangle \). Rotations of spin \( j \) about \( \pi/2 \) around the \( x \) and \( y \)-axis are basic QC operations. We will denote them by \( X_j \) and \( Y_j \) respectively. In matrix notation, they are given by

\[
X_j \equiv e^{i\pi S^x_j/2} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}, \tag{6}
\]

and

\[
Y_j \equiv e^{i\pi S^y_j/2} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}. \tag{7}
\]
Clearly operations such as (8) and (9) can be implemented in terms of the time evolution of model (3) by a proper choice of the model parameters. Writing $|a\rangle = a_0|00\rangle + a_1|10\rangle + a_2|01\rangle + a_3|11\rangle$ with $|b_1 b_2\rangle \equiv |b_1\rangle |b_2\rangle$ and $b_1, b_2 = 0, 1$ we have

$$X_1|a\rangle = X_1 \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i & 0 & 0 \\ i & 1 & 0 & 0 \\ 0 & 0 & 1 & i \\ 0 & 0 & i & 1 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix},$$

(8)

For example, $X_1|11\rangle = (|11\rangle + i|01\rangle)/\sqrt{2}$. Using the same labeling of the basis states as in (8) we have

$$Y_2 \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix},$$

(9)

e.g. $Y_2|11\rangle = (|10\rangle + |11\rangle)/\sqrt{2}$. The matrix expressions for the inverse of the rotations $X_1$ and $Y_2$, denoted by $X_1$ and $Y_2$ respectively, are obtained by taking the hermitian conjugates of the matrices in (8) and (9). For example, $Y_2|11\rangle = (|11\rangle - |10\rangle)/\sqrt{2}$.

**B. Two-qubit operations: CNOT gate**

Computation requires some form of communication between the qubits. A basic two-qubit operation is provided by the CNOT gate. The CNOT gate flips the second spin if the first spin is in the down state, i.e. the first qubit acts as a control qubit for the second one, see Table I. The procedure that we use to construct the CNOT gate may seem a little ad hoc and indeed to considerable extent it is. There is no unique method to construct QC gates.

On an ideal QC the CNOT gate can be implemented by a combination of single-qubit operations and a two-qubit phase shift operation $P$ defined by the matrix

$$P \equiv \begin{pmatrix} e^{i\phi_0} & 0 & 0 & 0 \\ 0 & e^{i\phi_1} & 0 & 0 \\ 0 & 0 & e^{i\phi_2} & 0 \\ 0 & 0 & 0 & e^{i\phi_3} \end{pmatrix}.$$ 

(10)

Assume that the QC is in a state

$$|\Psi\rangle = a_0|00\rangle + a_1|10\rangle + a_2|01\rangle + a_3|11\rangle.$$

(11)

First we apply to $|\Psi\rangle$ the rotation $Y_2$, as defined in (9). This gives

$$Y_2|\Psi\rangle = \frac{1}{\sqrt{2}}[(a_0 + a_2)|00\rangle + (a_1 + a_3)|10\rangle + (a_2 - a_0)|01\rangle + (a_3 - a_1)|11\rangle].$$

(12)

Next we apply to $Y_2|\Psi\rangle$ the phase shift $P$

$$PY_2|\Psi\rangle = \frac{1}{\sqrt{2}}[e^{i\phi_0}c_0|00\rangle + e^{i\phi_1}c_1|10\rangle + e^{i\phi_2}c_2|01\rangle + e^{i\phi_3}c_3|11\rangle],$$

(13)

where $c_0 = a_0 + a_2, c_1 = a_1 + a_3, c_2 = a_2 - a_0$ and $c_3 = a_3 - a_1$. Finally we apply the inverse of the rotation $Y_2$

$$Y_2^\dagger PY_2|\Psi\rangle = \frac{1}{2}[e^{i\phi_0}c_0 - e^{i\phi_2}c_2]|00\rangle + (e^{i\phi_1}c_1 - e^{i\phi_3}c_3)|10\rangle + (e^{i\phi_0}c_0 + e^{i\phi_2}c_2)|01\rangle + (e^{i\phi_1}c_1 + e^{i\phi_3}c_3)|11\rangle].$$

(14)

We now determine the angles $\phi_i$ such that the sequence (14) performs the CNOT operation. Since the CNOT gate will not change $a_0$ and $a_2$ (see Table I) we can choose $\phi_0 = \phi_2$. This gives

$$Y_2^\dagger PY_2|\Psi\rangle = e^{i\phi_0}[a_0|00\rangle + a_2|01\rangle + e^{i\beta}(a_1 \cos \alpha + i a_3 \sin \alpha)|10\rangle + e^{i\beta}(a_3 \cos \alpha + i a_1 \sin \alpha)|11\rangle],$$

(15)
where $\beta = \alpha + \phi_3 - \phi_0$ and $\alpha = (\phi_2 - \phi_3)/2$. The global phase factor $e^{i\phi_0}$ is physically irrelevant.

The simplest way to implement the phase shift $P$ is to use the time evolution, i.e. $P = e^{-i\tau H_I}$, of the Ising model

$$H_I = -JS_1^zS_2^z - hS_1^z - hS_2^z,$$

where the external fields acting on both spins are the same. From (16) it follows immediately that $\phi_0 = \tau(J/4 + h)$, $\phi_1 = \phi_2 = -\tau J/4$ and $\phi_3 = \tau(J/4 - h)$. Taking into account our choice $\phi_0 = \phi_2$, (15) becomes

$$\mathbf{Y}_2^2\mathbf{Y}_2 = e^{i\alpha/2}[a_0|00\rangle + a_2|01\rangle + e^{-ia}(a_1 \cos \alpha + ia_3 \sin \alpha)|10\rangle + e^{-ia}(a_3 \cos \alpha + ia_1 \sin \alpha)|11\rangle].$$

Using the same labeling of states as in (8) we have

$$\mathbf{Y}_2^2\mathbf{Y}_2 = e^{i\alpha/2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-ia} \cos \alpha & 0 & ie^{-ia} \sin \alpha \\ 0 & 0 & 1 & 0 \\ 0 & e^{-ia} \sin \alpha & 0 & e^{ia} \cos \alpha \end{pmatrix}.$$ 

Comparing the truth table of the CNOT gate (see Table I) with the matrix in (18), it is clear that putting $\alpha = \pi/2$ will do the job (upto an irrelevant global phase factor). In terms of Hamiltonian (16), $-\tau J = \pi$ and $h = -J/2$. The sequence

$$CNOT = \mathbf{Y}_2^2\mathbf{Y}_2 = e^{i\pi/4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

performs the CNOT operation on qubit 2 with qubit 1 acting as the control variable. Here we introduced the symbol $I$ to represent the time evolution $e^{-i\tau H_I}$ with $\tau = -\pi/J$.

C. Quantum Algorithms

Any QA can be written as a sequence of the one- and two-qubit operations discussed above. As a simple example of a QA we take $(CNOT)^5$. On an ideal QC, $CNOT^2$ is the identity operation and hence $(CNOT)^5 = CNOT$ but on a physical QC this is not always the case, see below. To illustrate the dependence of the quantum computation on the physical implementation and on the choice of the input state we consider two QA’s, $QA_1$ and $QA_2$, defined by

$$QA_1|b_1b_2\rangle \equiv (CNOT)^5|b_1b_2\rangle,$$

$$QA_2|\text{singlet}\rangle \equiv Y_1(CNOT)^5|\text{singlet}\rangle,$$

where $|\text{singlet}\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$. We have

$$\langle 01| - |11\rangle)/\sqrt{2} = (CNOT)^5|\text{singlet}\rangle,$$

and hence $\langle \text{singlet}|(CNOT)^5Q_1(CNOT)^5|\text{singlet}\rangle = 1/2$. We can obtain a clear-cut answer in terms of expectation values of the qubits by applying a $\pi/2$ rotation of spin 1

$$|11\rangle = Y_1(CNOT)^5|\text{singlet}\rangle.$$

Therefore in (21), the CNOT operations are followed by a $\pi/2$ rotation of spin 1.

As a more complicated example of a QA, we consider Grover’s database search algorithm to find the needle in a haystack. On a conventional computer, finding an item out of of $N$ elements requires $O(N)$ queries [13]. Grover has shown that a QC can find the item using only $O(\sqrt{N})$ attempts [2]. The reduction from $O(N)$ to $O(\sqrt{N})$ is due to the intrinsic massive parallel operation of the QC. Assuming a uniform probability distribution for the needle, for $N = 4$ the average number of queries required by a conventional algorithm is $9/4$ [16,14]. With Grover’s QA the correct answer can be found in a single query [14,16].

Experimentally Grover’s QA has been implemented on a 2-qubit NMR-QC for the case of a database containing four items [14,16]. In experiments [14,16] the sequences
have been chosen to implement Grover’s search algorithm. The subscript \( j \) of \( U_j \) corresponds to the position of the searched-for item in the database. In all four cases the input state is \(|00\rangle\). The two-qubit operation \( G \) is defined by

\[
G = \begin{pmatrix}
  e^{-i\pi/4} & 0 & 0 & 0 \\
  0 & e^{i\pi/4} & 0 & 0 \\
  0 & 0 & e^{i\pi/4} & 0 \\
  0 & 0 & 0 & e^{-i\pi/4}
\end{pmatrix},
\]

and performs a conditional phase shift.

On an ideal QC the QA’s (24) – (27) are by no means unique: Various alternative expressions can be written down by using the algebraic properties of the \( X \)’s and \( Y \)’s. This feature has been exploited to eliminate redundant elementary operations \([14]\). On an ideal QC sequences (24) – (27) return the correct answer, i.e. the position of the searched-for item. This is easily verified on the QCE by selecting the elementary operations that implement an ideal QC.

**IV. PHYSICAL QUANTUM COMPUTER**

**A. Single-qubit operations**

NMR uses SF pulses to rotate the spins. By tuning the frequency of the SF to the precession frequency of a particular spin (\( h^z \) in our case), the power of the applied pulse (= intensity times duration) controls how much the spin will rotate. The axis of the rotation is determined by the direction of the applied SF. The elementary model of a SF along the \( x \)-axis reads \([46]\)

\[
i \frac{\partial}{\partial t} |\Phi(t)\rangle = - \left( h^z_1 S^z_1 + \tilde{h}^z S^z_1 \sin \omega t \right) |\Phi(t)\rangle,
\]

where \( |\Phi\rangle = |\uparrow\rangle \langle \uparrow| + |\downarrow\rangle \langle \downarrow| \). \( |\Phi(t = 0)\rangle \) is the initial state of the two-state system and we have set the phase \( \phi_x = 0 \). Substituting \( |\Phi(t)\rangle = e^{i\tilde{h}^z t} |\Phi\rangle \) yields

\[
i \frac{\partial}{\partial t} |\Psi(t)\rangle = - \tilde{h}^z_1 (S^z_1 - \sin \omega t \cos \tilde{h}^z t + S^y_1 \sin \omega t \sin \tilde{h}^z t) |\Psi(t)\rangle.
\]

At resonance, i.e. \( \omega = \tilde{h}^z \), we find

\[
i \frac{\partial}{\partial t} |\Psi(t)\rangle = - \frac{\tilde{h}^y_1}{2} (S^y_1 + \sin 2\omega t - S^y_1 \cos 2\omega t) |\Psi(t)\rangle.
\]

Assuming that the effects of the higher harmonic terms (i.e. the terms in \( \sin 2\omega t \) and \( \cos 2\omega t \) are small \([46]\), \(31)\) is easily solved to give

\[
|\Psi(t)\rangle \approx e^{i 2 h^z_1 S^z_1 / 2} |\Psi(t = 0)\rangle,
\]

so that the overall action of a SF-pulse of duration \( \tau \) can be written as

\[
|\Phi(t + \tau)\rangle \approx e^{i \tilde{h}^z t S^z_1} e^{i \tilde{h}^z S^y_1 / 2} |\Phi(t)\rangle.
\]

Hence it follows that application of an SF-pulse of power \( \tau \tilde{h}^z = \pi \) will have the effect of rotating spin 1 by an angle of \( \pi / 2 \) about the \( y \)-axis, as is clear by comparing \(32)\) with \(33)\).

In deriving \(33)\), higher harmonics have been neglected, as indicated by the “\( \approx \)” sign. Instead of applying SF’s along the \( x \) or \( y \) direction, one may also consider using SF’s that rotate in the \( x-y \) plane. This leads to the TDSE \([47]\).
The result is \( \Phi(t) \in C^1(\mathbb{R} \to \mathbb{C}^{2N}) \) and instead of (33) we obtain

\[
|\Phi(t + \tau)\rangle = e^{i\tau h^z_1} e^{i\tau h^z_2} |\Phi(t)\rangle.
\]

A QC contains at least two spins. If in experiments it is difficult to shield a particular spin from the SF, an application of an SF pulse affects not only the state of the resonant spin but changes the state of the other spins too (unless they are perfectly aligned along the \( z \)-axis). A general analytical, quantitative analysis of this many-body problem is rather difficult. We will study the limiting case in which the interaction between the spins has negligible impact on the time evolution of the spins during application of the SF pulse. As our numerical results (see below) demonstrate, this is the case that is relevant to the model system considered in the present paper and also to experiments [14–17].

We consider the two-spin system described by the TDSE

\[
i \frac{\partial}{\partial t} |\Phi(t)\rangle = -\left[h^z_1 S^z_1 + h^z_2 S^z_2 + h^x_1 (S^y_1 \sin \omega t + S^y_2 \cos \omega t) + h^y_2 (S^x_2 \sin \omega t + S^x_1 \cos \omega t)\right] |\Phi(t)\rangle,
\]

Substituting \( |\Phi(t)\rangle = e^{i\omega(S^z_1 + S^z_2)} |\Psi(t)\rangle \) we obtain

\[
i \frac{\partial}{\partial t} |\Psi(t)\rangle = -\left[(h^z_1 - \omega) S^z_1 + (h^z_2 - \omega) S^z_2 + h^x_1 S^y_1 + h^y_2 S^y_2\right] |\Psi(t)\rangle.
\]

Our aim is to rotate spin 1 about an angle \( \phi_1 \) without affecting the state of spin 2. This can be accomplished as follows. First we choose

\[
\omega = h^z_1,
\]

i.e. the frequency of the SF pulse is tuned to the resonance frequency of spin 1. Then (37) can easily be integrated. The result is

\[
|\Phi(t)\rangle = e^{it(S^z_1 + S^z_2)} e^{ih^z_2 S^y_2} e^{ih^x_1 S^y_1} |\Phi(0)\rangle,
\]

where \( v_{n,m} \equiv (0, h^x_n, h^z_n - h^z_m) \).

The third factor in (43) rotates spin 2 around the vector \( v_{1,2} \). This factor can be expressed as

\[
e^{itS_m \cdot v_{n,m}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cos \frac{t|v_{n,m}|}{2} + i|v_{n,m}|^{-1} \begin{pmatrix} h^x_n & h^z_n - h^z_m \\ ih^x_m & h^z_m \end{pmatrix} \sin \frac{t|v_{n,m}|}{2},
\]

and we see that the SF pulse will not change the state of spin 2 if and only if the duration \( t_1 \) of the pulse satisfies

\[
t_1 |v_{1,2}| = t_1 \sqrt{(h^z_1 - h^z_2)^2 + (h^x_2)^2} = 4\pi n_1,
\]

where \( n_1 \) is a positive integer.

The second factor in (33) is a special case of (40). It is easy to see that if

\[
t_1 h^z_1 = \varphi_1,
\]

the second factor in (33) will rotate spin 1 about \( \varphi_1 \) around the \( y \)-axis. Therefore, if conditions (38), (41), and (42) are satisfied we can rotate spin 1 about \( \varphi_1 \) without affecting the state of spin 2, independent of the physical realization of the QC. However, the first factor in (34) can still generate a global phase shift. Although it drops out of the expression
of the expectation value of the qubits, in general it has to be taken into account in a QC calculation because this phase shift depends on the state of the spins. Adding the condition

$$t_1 h^z_1 = 4\pi k_1,$$

where $k_1$ is a positive integer ($h^z_1 > 0$ by definition), the first factor in [39] is always equal to one. Summarizing: If conditions (38), (41), (42), and (43) are satisfied we can rotate spin 1 about $\varphi_1$ without affecting the state of spin 2 and without introducing unwanted phase shifts.

A last constraint on the choice of the pulse parameters comes from the fact that

$$h_2^\alpha = \gamma h_1^\alpha, \quad \tilde{h}_2^\alpha = \gamma \tilde{h}_1^\alpha; \quad \alpha = x, y, z.$$  

Without loss of generality we will assume that $0 < \gamma < 1$, in concert with the choice of parameters [5].

Using constraint (44) and conditions (38), (41), (42), and (43) we have

$$(1 - \gamma)^2 k_1^2 + \frac{\gamma^2}{4} \left( \frac{\varphi_1}{2\pi} \right)^2 = n_1^2,$$  

and reversing the role of spin 1 and spin 2 we obtain

$$(1 - \frac{1}{\gamma})^2 k_2^2 + \frac{1}{4\gamma^2} \left( \frac{\varphi_2}{2\pi} \right)^2 = n_2^2,$$  

where $k_1$, $k_2$, $n_1$, and $n_2$ are positive integers. The angles of rotation about the $y$-axis can be chosen such that $0 \leq \varphi_1 \leq 2\pi$ and $0 \leq \varphi_2 \leq 2\pi$.

In general (45) or (46) have no solution but a good approximate solution may be obtained if $\gamma$ is a rational number and $k_1$ and $k_2$ are large. Let $\gamma = N/M$ where $N$ and $M$ are integers satisfying $0 < N < M$. It follows that the representation $k_1 = kMN^2$ and $k_2 = kNM^2$ will generate sufficiently accurate solutions of (45) and (46) if the integer $k$ is chosen such that

$$2kNM(M - N) \gg 1.$$  

In terms of $k$, $N$, and $M$, the relevant physical quantities are then given by

$$\frac{t_1 h^z_1}{2\pi} = 2kMN^2, \quad \frac{\tilde{h}_1^z}{h^z_1} = \frac{1}{2kMN^2} \frac{\varphi_1}{2\pi},$$  

and

$$\frac{t_2 h^z_2}{2\pi} = 2kM^3, \quad \frac{\tilde{h}_2^z}{h^z_2} = \frac{1}{2kM^3} \frac{\varphi_2}{2\pi}.$$  

In our numerical experiments we use (48) and (49) to determine the duration of the SF pulses for both the static and rotating SF’s. In the latter case the SF pulses will be optimized in the sense that a pulse that rotates spin 1 (2) will hardly affect spin 2 (1) if $k$ satisfies condition (53).

The assumption of a pure sinusoidal time dependence of the applied fields serves to simplify the analytical analysis given above. In experiment there is no good reason to stick to a simple time dependence of the pulses [48]. In general

$$i \frac{\partial}{\partial t} \Phi(t) = - \left[ h^z_1 S^z_1 + h^z_2 S^z_2 + w(t) \tilde{h}_1^z (S^x_1 \sin \omega t + S^y_1 \cos \omega t) + w(t) \tilde{h}_2^z (S^x_2 \sin \omega t + S^y_2 \cos \omega t) \right] \Phi(t),$$  

where $w(t)$ can be almost any waveform. For $\omega = h^z_1$, the formal solution of (50) reads

$$\Phi(t) = e^{i t h^z_1 (S^z_1 + S^z_2)} \exp \left( i \int_0^t du w(u) \tilde{h}_1^z S^y_1 \right) \exp \left( i \int_0^t du \left[ (h^z_2 - h^z_1) S^z_2 + w(u) \tilde{h}_2^z S^y_2 \right] \right) \Phi(0),$$  

where $\Phi(t)$ is the total wave function of the system, $w(t)$ is the applied waveform, and $\tilde{h}_1^z$ and $\tilde{h}_2^z$ are the time-dependent operators. We have

$$i \frac{\partial}{\partial t} \Phi(t)$$  

and

$$\frac{\partial}{\partial t} \Phi(t) = - \left[ h^z_1 S^z_1 + h^z_2 S^z_2 + w(t) \tilde{h}_1^z (S^x_1 \sin \omega t + S^y_1 \cos \omega t) + w(t) \tilde{h}_2^z (S^x_2 \sin \omega t + S^y_2 \cos \omega t) \right] \Phi(t).$$  

In our numerical experiments we use (48) and (49) to determine the duration of the SF pulses for both the static and rotating SF’s. In the latter case the SF pulses will be optimized in the sense that a pulse that rotates spin 1 (2) will hardly affect spin 2 (1) if $k$ satisfies condition (53).

The assumption of a pure sinusoidal time dependence of the applied fields serves to simplify the analytical analysis given above. In experiment there is no good reason to stick to a simple time dependence of the pulses [48]. In general
where \( \exp \{ \ldots \} \) denotes the time-ordered exponential. The introduction of a general form of \( w(t) \) replaces condition (41) by

\[
\exp \left\{ i \int_0^{t_1} du \left[ (h_2^z - h_1^z)S_2^z + w(u)\tilde{h}_2^z S_2^z \right] \right\} = 1,
\]

and condition (42) becomes

\[
t_1\tilde{h}_1^z \int_0^{t_1} du \, w(u) = \varphi_1,
\]

expressing the fact that the rotation angle \( \varphi_1 \) is determined by the power of the pulse only. Conditions (43) and (44) remain the same. There are many forms of \( w(u) \) that will satisfy (53), so in this respect there is a lot of freedom in the choice of \( w(t) \). Finding the form of \( w(u) \) such that also (52) holds is a (complicated) optimization problem, in particular when the QC contains several qubits.

To summarize: If conditions (38), (41), (42), and (43) are satisfied we can rotate spin 1 about \( X \), \( Y \), and \( Z \) respectively. For integer \( j \) and condition (45) becomes

\[
\exp \left\{ i \left( \int_0^{t_1} du \phi u \right) \right\} = 1
\]

or

\[
\exp \left\{ i \left( \int_0^{t_1} du \phi \right) \right\} = 1
\]

For our choice (5) of the model parameters, \( \gamma = 1/4 \) such that \( N = 1 \) and \( M = 4 \). In general \( \gamma \) will not be a ratio of two small integers but it may be approximated to any desired precision by a rational number. Let us consider the hypothetical case \( N = 11, M = 40 \) such that \( \gamma = 11/40 = 0.275 \). Then (57) reads 25520k \( \gg 1 \) so that the choice \( k = 1 \) already yields an accurate solution to (47) and (48). However as \( t_{1}h_{2}^z/2\pi = 9680 \) and \( t_{2}h_{2}^z/2\pi = 128000 \), rather long SF pulses are required to perform these nearly ideal, single-qubit operations. As this example shows, the duration of the pulses that implement accurate single-qubit operations will be determined by the representation of \( \gamma \) as a ratio of two (small) integers.

From (58) and (59) it follows that \( |\tilde{h}_1^z| \ll |\tilde{h}_2^z| \) for accurate single-qubit operations. This implies \( t_{1}h_{1}^z(1 - \gamma) = 4\pi n_{1} \) or \( k_{1}(M - N) = M n_{1} \). For \( N = 1 \) and \( M = 4 \) we see that \( k_{1} \) has to be a multiple of 4. This reasoning readily generalizes: For \( n \) spins \( k_{1}(M_{j} - N_{j}) = M_{j} n_{j} \) for integer \( n_{j} \) and \( j = 2, \ldots, n \). In other words, the frequencies of precession of each of the qubits have to be commensurate with each other. Otherwise systematic phase errors will be generated in the course of the computation. This conclusion does not depend on the peculiarities of the NMR technique: It holds in general.

**B. Two-qubit operations: CNOT gate**

As the CNOT sequence (19) has been constructed on the basis of model (16), some modification is necessary to account for the fact that the two nuclear spins feel different static fields (see (4)). In general the Hamiltonian reads

\[
H_{NMR} = -JS_{1}^z S_{2}^z - h_{1}^z S_{1}^z - h_{2}^z S_{2}^z.
\]

Comparison of (23) with (54) shows that the implementation of the CNOT operation requires additional rotations:

\[
\text{CNOT} = \prod_{2} e^{-i\tau(h_{2}^z-h_{1}^z)S_{1}^z} e^{-i\tau(h_{2}^z-h_{1}^z)S_{2}^z} e^{-i\tau H_{NMR} Y_{2}},
\]

where we used the fact that \( Y_{2} \prod_{2} = 1 \). The extra phase shifts in (55) can be expressed in terms of single-qubit operations. The identities

\[
e^{-i\tau(h_{2}^z-h_{1}^z)S_{1}^z} = Y_{1}X_{1}^{\prime}Y_{1} = X_{1}Y_{1}^{\prime}X_{1},
\]

\[
e^{-i\tau(h_{2}^z-h_{1}^z)S_{2}^z} = Y_{2}X_{2}^{\prime}Y_{2},
\]

define the single-spin rotations \( X_{1}^{\prime}, Y_{1}^{\prime}, \) and \( Y_{2}^{\prime} \).

As (56) and (57) suggest, there are many different, logically equivalent sequences that implement the CNOT gate on an NMR QC. We have chosen to limit ourselves to the representations

\[
\text{CNOT}_{1} = Y_{1}X_{1}^{\prime}Y_{1}^{-1}X_{2}^{\prime}Y_{2}^{-1}I' Y_{2},
\]

\[
\text{CNOT}_{2} = Y_{1}X_{1}^{\prime}X_{2}^{\prime}I' Y_{1} Y_{2},
\]

\[
\text{CNOT}_{3} = X_{1}Y_{1}^{\prime}X_{2}^{\prime}Y_{2}^{-1}X_{1}I' Y_{2},
\]
where we introduced the symbol \( I' \) to represent the time evolution \( e^{-i\tau H_{NMR}} \) with \( \tau = -\pi/J \). On an ideal QC the sequences (53) – (60) give identical results. On an NMR-like QC they do not because operations such as \( X_1 \) and \( X_2 \) no longer commute. We will use sequences (58) – (60) to demonstrate the QPP.

### C. Quantum Algorithms

On a conventional computer an algorithm is a sequence of logical operations that defines a one-to-one relation between the input and output data. We expect that a conventional computer always returns the correct result, irrespective of the input. Also a QC should have correct (input, output) relationships. In contrast to a conventional computer, a QC accepts as input linear superpositions of basis states and can return superpositions as well. If a quantum gate correctly operates on each of the basis states, it will also do so on any general linear superposition unless the operation generates additional phase factors that depend on the input state. Of course this does not happen on an ideal QC but on a realistic one it may. Above we have shown how to reduce unwanted phase errors that result from imperfections of the one- and two-qubit operations.

For each realization of QC hardware, there is a one-to-one correspondence between the QA and the unitary matrix that transforms the superposition accordingly. A QA will operate correctly under all circumstances if the whole unitary matrix representing the QA is a good approximation to the ideal one. In other words, the magnitude and the phase of all matrix elements should be close to their ideal values. It is not sufficient to have for example two different CNOT gates that operate correctly by themselves: Also the relative phases that they produce should match. For \( n \) qubits there are \( 2^n(2^n - 1) \) real numbers that specify the unitary matrix corresponding to a QA. All these numbers should be close to their ideal values, otherwise the QA is bound to produce wrong answers.

Experimental realizations of QC’s have not yet demonstrated that a QC can correctly compute the answer for inputs other than simple basis states. However, with the QC hardware currently available such a test is definitely within reach. The two simple QA’s, (20) and (21) may be used for this purpose. In general on a physical QC, \( CNOT^2 \neq 1 \) and hence \((CNOT)^5\) in (20) and (21) does not reduce to one CNOT operation. The effect of the physical implementation of a QC on the logical operation of a QA will be most clear unless the operation generates additional phase factors that depend on the input state. Of course this does not happen on an ideal QC but on a realistic one it may. Above we have shown how to reduce unwanted phase errors that result from imperfections of the one- and two-qubit operations.

In the case of Grover’s database search algorithm, the representation of \( G \) in terms of the time evolution of (54) reads

\[
G = e^{-i\pi S_1 S_2} = e^{-i\tau h_1^i S_1} e^{-i\tau h_2^i S_2} e^{-i\tau H_{NMR}} = Y_2 X_2' Y_1 X_1' e^{-i\tau H_{NMR}},
\]

where \( \tau = -\pi/J \). This choice of \( \tau \) also fixes the angles the rotations, and through relations (58) and (59) also all parameters of the operations \( X_1' \) and \( X_2'' \).

### V. SIMULATION

#### A. Model parameters

The parameters of model (1) for which \( e^{-i\tau H} \) implements the EO’s of the ideal QC are listed in Table I. On an NMR-like QC, the one-qubit operations can be implemented by applying SF pulses, as explained above. The two-qubit operation \( I' \) can be implemented by letting the system evolve in time according to Hamiltonian \( H_{NMR} \), given by (54). \( I' \) is the same for both an ideal or NMR-like QC. Note that the condition \( \tau J = -\pi \) yields \( \tau/2\pi = 1162790.6977 \), a fairly large number (compared to our reference \( h_i^1 = 1 \), see (3)).

The model parameters for the fixed and rotating SF’s are determined according to the theory outlined above. We use the integer \( k \) to compute all free parameters and the subscript \( s = 2kMN^2 \) to label the results of the QC calculation. For reference we present the set of parameters corresponding to \( k = 1 \) for QC’s using fixed and rotating SF in Tables III and IV respectively.
B. Results

As a standard test we execute all sequences on an implementation of the ideal QC (see Table \[4\]). They all give the exact answers (results not shown). Furthermore the results (not shown) do not change if we put \( J = 0 \) in all single-qubit operations, which is not a surprise in view of the fact that typical pulse durations are much smaller than \( 1/2|J| \). It is also necessary to rule out that the numerical results depend on the time step \( \delta \) used to solve the TDSE. The numerical error of the product formula used by QCE is proportional to \( \delta^2 \) \[11\] [13]. It goes down by a factor of about one hundred if we reduce the time step by a factor of 10. Within the two-digit accuracy used to present our data, there is no difference between the results for \( \delta = 0.01 \) and \( \delta = 0.001 \). Hence we can be confident that we are solving the TDSE with a sufficiently high accuracy.

In Table \[V\] we present simulation results for QA’s, \( QA_1 \) and \( QA_2 \) defined by (20) and (23) respectively. It is clear that even the least accurate implementation \((s = 8, k = 1)\) nicely reproduces the correct answers if the input corresponds to one of the four basis states. The corresponding entries for \( QA_2 \) seem to suggest that \( CNOT_1 \) is working well for \( s = 8 \). However the result for \( s = 16 \) \((k = 2)\) shows that the apparently good result for \( s = 8 \) is accidental, as we might have expected on the basis of criterion \((47)\) (which in this case reads \( 24 \gg 1 \)). In agreement with the theoretical analysis of Section \[IV.A\] the results converge to the exact ones for sufficiently large \( k \), as shown in Table \[V\]. For small \( s \), the difference in the accuracy with which \( QA_1 \) and \( QA_2 \) give the correct answer clearly shows that in order for a QA to work properly, it is not sufficient to show that it correctly operates only when the input corresponds to one of the basis states.

In the regime where phase errors are significant the QA’s exhibit the QPP. This is exemplified in Tables \[VI\] and \[VII\] where we show the results of using \( CNOT_2 \) and \( CNOT_3 \) instead of \( CNOT_1 \). For \( k < 32 \) there is a clear signature of the QPP: These logically identical QA’s are sensitive to the order in which the single-qubit operations are carried out.

The results presented in Tables \[V\]–\[VII\] have been obtained using rotating SF’s. As explained above, in this case a single-qubit operation on qubit \( j \) exactly rotates qubit \( j \) about the specified angle (but perturbs the state of the other spin). In Table \[VIII\] we present simulation results obtained by using SF in the \( x \) or \( y \) direction only. Then the single-spin rotation on spin \( j \) no longer corresponds to the exact one. Nevertheless, as Table \[VIII\] shows, for sufficiently large \( s \) the results nicely converge to the correct answers. Apparently, for a QA to compute correctly, it is more important to have the phase errors under control than to perform very accurate single-spin rotations.

The very essence of QA’s is the use of entangled states at some stage of the calculations. It is at this point that the QA is most sensitive to (accumulated) phase errors. As another illustration of this phenomenon, we present in Tables \[IX\] and \[X\] some typical results obtained by executing Grover’s database search algorithm on the same model QC’s as those used in the examples discussed above. We find that reasonably good answers are obtained if \( s \geq 32 \), in concert with the observations based on QA’s \( QA_1 \) and \( QA_2 \).

The results discussed above show effects of imperfections in the physical implementation of single-qubit operations. Thereby we assumed that \( J \), and the static applied fields \( h_1 \) and \( h_2 \) are fixed in time and known to very high precision. The Ising-model time evolution was used to perform two-qubit operations, leaving only the duration of this operation as a possible source for causing errors. In Table \[XI\] we give examples of the extreme sensitivity of a QA to the precision with which the parameters have to be specified. Essentially we repeated the calculation of Table \[V\] for \( s = 256 \) but on purpose we made an error in the specification of the duration of \( I' \). As Table \[XI\] shows, an error in the 8-th digit can have a devastating effect on the outcome of the QC calculation. This again is just another manifestation of the QPP but not really a surprise: During the application of \( I' \) the spins rotate around the \( z \)-axis with their resonance frequencies \( h_1 \) and \( h_2 \). A small deviation in \( \tau/2\pi \) from its ideal value produces phase errors. Note however that the integer part of \( \tau/2\pi \) is also essential to perform the correct conditional phase shift. Therefore, in practice it is necessary to specify the duration of the time evolution \( I' \) to at least 8 digits (for the case \( |J|/h_1 \approx 10^{-6} \)).

VI. SUMMARY

On a physically realizable, non-ideal quantum computer, operations that manipulate one particular qubit also affect the state of other qubits. This may cause unwanted deviations from the ideal motion of the total system and lead to practical problems of programming quantum computers: An implementation of a quantum computation that works well on one quantum computer may fail on others.

We have classified the various physical sources that lead to deviations. The most obvious one originates from the fact that other spins cannot be kept still during an operation on one particular spin. If these spins do not return to their original state when this operation is over, the quantum computation is unlikely to give correct answers \[13\].
Proper optimization of the parameters that control the single-qubit operations can largely eliminate this source of errors. However, even if the operation gives almost exact results for all basis states, the operation is not necessarily perfect. That is, the operation generally yields a global phase factor which depends on the input states. Therefore, when such an operation is applied on a linear combination of the basis states, the relative phases of the basis states change, resulting in incorrect quantum computation. This is a second source for deviations from correct quantum computer operation.

We have derived additional conditions on the parameters that control the single-qubit operations and have obtained the conditions for reliable quantum computation. Unfortunately, these conditions cannot be satisfied simultaneously. However they can be satisfied to any precision by increasing the duration of the single-qubit operations. Using the controlled-NOT gate and Grover’s search algorithm as examples, we have given concrete demonstrations of how the above mentioned problems arise and how they can be solved.

At this moment, we do not know how to stabilize the quantum computation by controlling the evolution of the state of a closed quantum system. In a classical computer the presence of dissipation enables reliable computation. However, dissipation seems detrimental for quantum computer operation. Therefore, at this moment, the only option is to perform each operation as perfect as possible. The present paper shows how this may be done.

The condition on the commensurability of the precession frequencies of the individual qubits leads to an increase of the execution time of single-qubit operations. Unless the precession frequencies of the qubits are the same to great precision, the execution time will grow rapidly with the number of qubits and substantially limit the speed of quantum computation. Therefore new techniques have to be developed to compensate for this loss in efficiency. Quantum error correction schemes that work well on an ideal quantum computer require many extra qubits and many additional operations to detect and correct errors. On a physical quantum computer however, the error-correction qubits will suffer from the same deficiencies as those exposed in this paper. Possibly, the clever use of dissipation processes may help to perform automatic error correction [49]. All this puts considerable demands on the technology to fabricate qubits. It remains a great challenge to demonstrate that a QC of many qubits can perform a genuine computation in less time than a conventional computer.

ACKNOWLEDGEMENT

Support from the Dutch “Stichting Nationale Computer Faciliteiten (NCF)” and the Grant-in-Aid from the Japanese Ministry of Education, Science, Sports and Culture is gratefully acknowledged.
TABLE I. Input and output states and the corresponding expectation values \((a, b)\) of the qubits for the CNOT operation.

| Input state | \(a\) | \(b\) | Output state | \(a\) | \(b\) |
|-------------|-------|-------|--------------|-------|-------|
| \(|00\rangle\) | 0     | 0     | \(|00\rangle\) | 0     | 0     |
| \(|10\rangle\) | 1     | 0     | \(|11\rangle\) | 1     | 1     |
| \(|01\rangle\) | 0     | 1     | \(|01\rangle\) | 0     | 1     |
| \(|11\rangle\) | 1     | 1     | \(|10\rangle\) | 1     | 0     |

TABLE II. Model parameters for the elementary operations on the ideal QC. Parameters of model (3) that do not appear in this table are zero, except for the interaction \(J = -0.43 \times 10^{-6}\). The TDSE is solved using a time step \(\delta/2\pi = 1\).

| \(\tau / 2\pi\) | \(h^x_1\) | \(h^y_1\) | \(h^z_1\) | \(h^x_2\) | \(h^y_2\) | \(h^z_2\) |
|----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| \(X_1\)       | 0.25      | 1         | 0         | 0         | 0         | 0         |
| \(X_2\)       | 0.25      | 0         | 1         | 0         | 0         | 0         |
| \(Y_1\)       | 0.25      | 0         | 0         | 1         | 0         | 0         |
| \(Y_2\)       | 0.25      | 0         | 0         | 0         | 1         | 0         |
| \(X'_1\)      | 1         | -0.4477   | 0         | 0         | 0         | 0         |
| \(X'_2\)      | 1         | 0         | -1.4244   | 0         | 0         | 0         |
| \(Y'_1\)      | 1         | 0         | 0         | 0.4477    | 0         | 0         |
| \(Y'_2\)      | 1         | 0         | 0         | 0         | 0         | 0         |
| \(X''_1\)     | 1         | -0.6977   | 0         | 0         | 0         | 0         |
| \(X''_2\)     | 1         | 0         | -1.6744   | 0         | 0         | 0         |
| \(I\)         | \(-1/2J\) | 0         | 0         | 0         | \(-J/2\) | \(-J/2\) |
| \(I'\)        | \(-1/2J\) | 0         | 0         | 0         | 1         | 0.25      |
| \(G\)         | \(-1/2J\) | 0         | 0         | 0         | 1         | 0.25      |

TABLE III. Model parameters of single-qubit operations on an NMR QC for the case \((k = 1, N = 1, M = 4)\), see (48) and (49). Parameters of model (3) that do not appear in this table are zero, except for the interaction \(J = -0.43 \times 10^{-6}\) and the constant magnetic fields \(h^z_1 = 1\) and \(h^z_2 = 0.25\). The TDSE is solved using a time step \(\delta/2\pi = 0.01\).

| \(\tau / 2\pi\) | \(\omega\) | \(\hat{h}^x_1\) | \(\hat{h}^y_1\) | \(\hat{h}^z_1\) | \(\hat{h}^x_2\) | \(\hat{h}^y_2\) | \(\hat{h}^z_2\) |
|----------------|------------|---------------|---------------|---------------|---------------|---------------|---------------|
| \(X_1\)       | 8          | 1.00          | 0             | 0             | -0.0625000    | -0.0156250    | -0.0156250    |
| \(X_2\)       | 128        | 0.25          | 0             | 0             | -0.0156250    | -0.0039063    | -0.0039063    |
| \(Y_1\)       | 8          | 1.00          | 0.0625000     | 0.0156250     | 0             | 0             | 0             |
| \(Y_2\)       | 128        | 0.25          | 0.0156250     | 0.0039063     | 0             | 0             | 0             |
| \(X'_1\)      | 8          | 1.00          | 0             | 0             | 0.1119186     | 0.0279796     | 0.0279796     |
| \(X'_2\)      | 128        | 0.25          | 0             | 0             | 0.0890262     | 0.0222565     | 0.0222565     |
| \(Y'_1\)      | 8          | 1.00          | -0.1119186    | -0.0279796    | 0             | 0             | 0             |
| \(Y'_2\)      | 8          | 1.00          | 0             | 0             | 0.1744186     | 0.0436046     | 0.0436046     |
| \(X''_1\)     | 128        | 0.25          | 0             | 0             | 0.1046512     | 0.0261628     | 0.0261628     |
TABLE IV. Model parameters of single-qubit operations on an NMR QC using rotating SF’s for the case \((k = 1, N = 1, M = 4)\), see \((38)\) and \((39)\). Parameters of model \((3)\) that do not appear in this table are zero, except for the interaction \(J = -0.43 \times 10^{-9}\) and the constant magnetic fields \(h_{1x}^1 = 1\) and \(h_{2x}^2 = 0.25\). The TDSE is solved using a time step \(\delta/2\pi = 0.01\).

| \(\tau/2\pi\) | \(\omega\) | \(h_{1x}^1\) | \(h_{2x}^2\) | \(\varphi_{x}\) | \(h_{1y}^1\) | \(h_{2y}^2\) | \(\varphi_{y}\) |
|-------------|------|-----------|-----------|-------------|-----------|-----------|-------------|
| \(X_1\)     | 8    | -0.0312500 | -0.0078125 | -\(\pi/2\)  | -0.0312500 | -0.0078125 | 0           |
| \(X_2\)     | 128  | -0.0078125 | -0.0039063 | -\(\pi/2\)  | -0.0078125 | -0.0039063 | 0           |
| \(Y_1\)     | 8    | 1.00       | 0.0156250 | 0           | 0.0312500  | 0.0156250  | \(\pi/2\)   |
| \(Y_2\)     | 128  | 0.25       | 0.0039063 | 0           | 0.0078125  | 0.0039063  | \(\pi/2\)   |
| \(X_1'\)    | 8    | 1.00       | 0.0559593 | -\(\pi/2\)  | 0.0559593  | 0.0139898  | 0           |
| \(X_2'\)    | 128  | 0.25       | 0.0445131 | -\(\pi/2\)  | 0.0445131  | 0.011283   | 0           |
| \(Y_1'\)    | 8    | 1.00       | -0.0559593| 0           | -0.0559593 | 0.0139898  | \(\pi/2\)   |
| \(X_2''\)   | 8    | 1.00       | 0.0872093 | -\(\pi/2\)  | 0.0872093  | 0.0218023  | 0           |
| \(X_2''\)   | 128  | 0.25       | 0.0523256 | -\(\pi/2\)  | 0.0523256  | 0.0130914  | 0           |

TABLE V. Expectation values of the two qubits as obtained by performing a sequence of five CNOT operations on a QC that uses rotating SF’s to manipulate individual qubits. The initial states \([10], [01], [11]\), and \([\text{singlet}] = (|01\rangle - |10\rangle)/\sqrt{2}\) have been prepared by starting from the state \([00]\) and performing exact rotations of the spins. The CNOT operations on the singlet state are followed by a \(\pi/2\) rotation of spin 1 to yield a non-zero value of qubit 1. The subscripts in \(a_s\) and \(b_s\) refer to the time \(s = \tau/2\pi = 2kMN^2\) and determine the duration and strength of the SF pulses through relations \((38)\) and \((39)\), see Table \([X]\) for the example of the case \(s = 8\). The CNOT operation itself was implemented by applying sequence CNOT\(_1\) given by \((38)\). On an ideal QC, CNOT\(_1\) is the identity operation. The results obtained on an ideal QC are given by \(a\) and \(b\).

| Operation | \(a\) | \(b\) | \(a_8\) | \(b_8\) | \(a_{16}\) | \(b_{16}\) | \(a_{32}\) | \(b_{32}\) | \(a_{64}\) | \(b_{64}\) | \(a_{256}\) | \(b_{256}\) |
|-----------|------|------|-------|-------|--------|--------|--------|--------|--------|--------|--------|--------|
| \((\text{CNOT}_1)^5|00\rangle\) | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| \((\text{CNOT}_1)^5|10\rangle\) | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| \((\text{CNOT}_1)^5|01\rangle\) | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 |
| \((\text{CNOT}_1)^5|11\rangle\) | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 |
| \(Y_1(\text{CNOT}_1)^5|\text{singlet}\rangle\) | 1.00 | 1.00 | 0.90 | 1.00 | 0.03 | 1.00 | 0.58 | 1.00 | 0.88 | 1.00 | 0.99 | 1.00 |

TABLE VI. Same as Table \(V\) except that instead of CNOT\(_1\) sequence CNOT\(_2\) given by \((54)\) was used to perform the quantum computation.

| Operation | \(a\) | \(b\) | \(a_8\) | \(b_8\) | \(a_{16}\) | \(b_{16}\) | \(a_{32}\) | \(b_{32}\) | \(a_{64}\) | \(b_{64}\) | \(a_{256}\) | \(b_{256}\) |
|-----------|------|------|-------|-------|--------|--------|--------|--------|--------|--------|--------|--------|
| \((\text{CNOT}_2)^5|00\rangle\) | 0.00 | 0.00 | 0.24 | 0.76 | 0.50 | 0.26 | 0.20 | 0.07 | 0.06 | 0.02 | 0.00 | 0.00 |
| \((\text{CNOT}_2)^5|10\rangle\) | 1.00 | 1.00 | 0.76 | 0.24 | 0.50 | 0.74 | 0.80 | 0.93 | 0.95 | 0.98 | 1.00 | 1.00 |
| \((\text{CNOT}_2)^5|01\rangle\) | 0.00 | 1.00 | 0.24 | 0.24 | 0.51 | 0.74 | 0.20 | 0.93 | 0.06 | 0.98 | 0.00 | 1.00 |
| \((\text{CNOT}_2)^5|11\rangle\) | 1.00 | 0.00 | 0.76 | 0.76 | 0.50 | 0.26 | 0.80 | 0.07 | 0.95 | 0.02 | 1.00 | 0.00 |
| \(Y_1(\text{CNOT}_2)^5|\text{singlet}\rangle\) | 1.00 | 1.00 | 0.98 | 0.24 | 0.95 | 0.74 | 0.98 | 0.93 | 0.99 | 0.98 | 1.00 | 1.00 |
TABLE VII. Same as Table V except that instead of $CNOT_1$ sequence $CNOT_3$ given by (20) was used to perform the quantum computation.

| Operation | $a$ | $b$ | $a_8$ | $b_8$ | $a_{16}$ | $b_{16}$ | $a_{32}$ | $b_{32}$ | $a_{64}$ | $b_{64}$ | $a_{256}$ | $b_{256}$ |
|-----------|-----|-----|-------|-------|----------|----------|----------|----------|----------|----------|----------|----------|
| $(CNOT_3)^5|00⟩$ | 0.00 | 0.00 | 0.23 | 0.76 | 0.50 | 0.26 | 0.20 | 0.07 | 0.06 | 0.02 | 0.00 | 0.00 |
| $(CNOT_3)^5|10⟩$ | 1.00 | 1.00 | 0.77 | 0.24 | 0.50 | 0.74 | 0.80 | 0.93 | 0.95 | 0.98 | 1.00 | 1.00 |
| $(CNOT_3)^5|01⟩$ | 0.00 | 1.00 | 0.23 | 0.24 | 0.51 | 0.74 | 0.20 | 0.93 | 0.06 | 0.98 | 0.00 | 1.00 |
| $(CNOT_3)^5|11⟩$ | 1.00 | 0.00 | 0.77 | 0.24 | 0.26 | 0.50 | 0.80 | 0.97 | 0.95 | 0.02 | 1.00 | 0.00 |
| $Y_1(CNOT_3)^5|\text{singlet}⟩$ | 1.00 | 1.00 | 0.00 | 1.00 | 0.79 | 0.24 | 0.55 | 0.93 | 0.20 | 0.93 | 0.06 | 0.98 |
| $Y_1(CNOT_3)^5|\text{singlet}⟩$ | 1.00 | 1.00 | 0.00 | 1.00 | 0.79 | 0.24 | 0.55 | 0.93 | 0.20 | 0.93 | 0.06 | 0.98 |

TABLE VIII. Same as Table V except that instead of rotating SF’s, SF’s along either the $x$ or $y$-axis were used to manipulate individual qubits. See Table III for the example of the set of model parameters for $s = 8$.

| Operation | $a$ | $b$ | $a_8$ | $b_8$ | $a_{16}$ | $b_{16}$ | $a_{32}$ | $b_{32}$ | $a_{64}$ | $b_{64}$ | $a_{256}$ | $b_{256}$ |
|-----------|-----|-----|-------|-------|----------|----------|----------|----------|----------|----------|----------|----------|
| $(CNOT_1)^5|00⟩$ | 0.00 | 0.00 | 0.00 | 0.03 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| $(CNOT_1)^5|10⟩$ | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| $(CNOT_1)^5|01⟩$ | 0.00 | 1.00 | 0.00 | 0.97 | 0.00 | 0.99 | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 |
| $(CNOT_1)^5|11⟩$ | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 | 1.00 | 0.00 |
| $Y_1(CNOT_1)^5|\text{singlet}⟩$ | 1.00 | 1.00 | 0.02 | 0.98 | 0.45 | 1.00 | 0.17 | 1.00 | 0.70 | 1.00 | 0.98 | 1.00 |

TABLE IX. Expectation values of the two qubits as obtained by running Grover’s database search algorithm on a QC that uses rotating SF’s to manipulate individual qubits. The subscripts in $a_s$ and $b_s$ refer to the time $s = \tau / 2\pi = 2kMN^2$ and determine the duration and strength of the SF pulses through relations (48) and (49), see Table IV for the example of the case $s = 8$. The results obtained on an ideal QC are given by $a$ and $b$.

| Item position | $a$ | $b$ | $a_8$ | $b_8$ | $a_{16}$ | $b_{16}$ | $a_{32}$ | $b_{32}$ | $a_{64}$ | $b_{64}$ | $a_{256}$ | $b_{256}$ |
|---------------|-----|-----|-------|-------|----------|----------|----------|----------|----------|----------|----------|----------|
| 0             | 0.00 | 0.00 | 0.48 | 0.53 | 0.15 | 0.16 | 0.04 | 0.04 | 0.01 | 0.01 | 0.00 | 0.00 |
| 1             | 1.00 | 0.00 | 0.52 | 0.50 | 0.85 | 0.15 | 0.96 | 0.04 | 0.99 | 0.01 | 1.00 | 1.00 |
| 2             | 0.00 | 1.00 | 0.55 | 0.48 | 0.15 | 0.84 | 0.04 | 0.96 | 0.01 | 0.99 | 0.00 | 1.00 |
| 3             | 1.00 | 1.00 | 0.45 | 0.50 | 0.85 | 0.85 | 0.96 | 0.96 | 0.99 | 0.99 | 1.00 | 0.00 |

TABLE X. Same as Table IX except that instead of rotating SF’s, SF’s along either the $x$ or $y$-axis were used to manipulate individual qubits. See Table III for the example of the set of model parameters for $s = 8$.

| Item position | $a$ | $b$ | $a_8$ | $b_8$ | $a_{16}$ | $b_{16}$ | $a_{32}$ | $b_{32}$ | $a_{64}$ | $b_{64}$ | $a_{256}$ | $b_{256}$ |
|---------------|-----|-----|-------|-------|----------|----------|----------|----------|----------|----------|----------|----------|
| 0             | 0.00 | 0.00 | 0.92 | 0.91 | 0.39 | 0.35 | 0.11 | 0.10 | 0.03 | 0.03 | 0.00 | 0.00 |
| 1             | 1.00 | 0.00 | 0.09 | 0.91 | 0.61 | 0.36 | 0.89 | 0.10 | 0.97 | 0.03 | 1.00 | 1.00 |
| 2             | 0.00 | 1.00 | 0.95 | 0.10 | 0.36 | 0.65 | 0.10 | 0.90 | 0.03 | 0.98 | 0.00 | 1.00 |
| 3             | 1.00 | 1.00 | 0.05 | 0.09 | 0.64 | 0.64 | 0.90 | 0.90 | 0.97 | 0.97 | 1.00 | 0.00 |
TABLE XI. Same as Table V except for a change in the duration of the operation \( I' \). \( (a^{(1)}_{256}, b^{(1)}_{256}) \): \( \tau/2\pi = 1162790.4977 \); \( (a^{(2)}_{256}, b^{(2)}_{256}) \): \( \tau/2\pi = 1162790.5977 \); \( (a^{(3)}_{256}, b^{(3)}_{256}) \): \( \tau/2\pi = 1162790.6977 \) (correct value); \( (a^{(4)}_{256}, b^{(4)}_{256}) \): \( \tau/2\pi = 1162790.7977 \); \( (a^{(5)}_{256}, b^{(5)}_{256}) \): \( \tau/2\pi = 1162790.8977 \).

| Operation       | \( a \) | \( b \) | \( a^{(1)}_{256} \) | \( b^{(1)}_{256} \) | \( a^{(2)}_{256} \) | \( b^{(2)}_{256} \) | \( a^{(3)}_{256} \) | \( b^{(3)}_{256} \) | \( a^{(4)}_{256} \) | \( b^{(4)}_{256} \) | \( a^{(5)}_{256} \) | \( b^{(5)}_{256} \) |
|-----------------|--------|--------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| \((CNOT_1)^{[00]}\) | 0.00   | 0.00   | 0.00           | 0.52           | 0.00           | 0.16           | 0.00           | 0.00           | 0.00           | 0.13           | 0.00           | 0.48           |
| \((CNOT_1)^{[10]}\) | 1.00   | 1.00   | 1.00           | 0.48           | 1.00           | 0.87           | 1.00           | 1.00           | 1.00           | 0.84           | 1.00           | 0.48           |
| \((CNOT_1)^{[01]}\) | 0.00   | 1.00   | 0.00           | 0.48           | 0.00           | 0.84           | 0.00           | 0.00           | 0.00           | 0.87           | 0.00           | 0.52           |
| \((CNOT_1)^{[11]}\) | 1.00   | 0.00   | 1.00           | 0.52           | 1.00           | 0.13           | 1.00           | 1.00           | 1.00           | 0.16           | 1.00           | 0.52           |
| \(Y_1(CNOT_1)^{[\text{singlet}]}\) | 1.00   | 1.00   | 0.99           | 0.50           | 0.09           | 0.85           | 0.99           | 1.00           | 0.01           | 0.85           | 0.99           | 0.50           |
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