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# Quantum Spin Dynamics and Quantum Computation

H. De Raedt[1,*], A.H. Hams[1], K. Michielsen[2], S. Miyashita[3] and K. Saito[3]

[1]*Institute for Theoretical Physics and Materials Science Centre*
[2]*Laboratory for Biophysical Chemistry*
*University of Groningen, Nijenborgh 4*
*NL-9747 AG Groningen, The Netherlands*

[3]*Department of Applied Physics, School of Engineering*
*University of Tokyo, Bunkyo-ku, Tokyo 113*

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We describe a simulation method for a quantum spin model of a generic, general purpose quantum computer. The use of this quantum computer simulator is illustrated through several implementations of Grover's database search algorithm. Some preliminary results on the stability of quantum algorithms are presented.

KEYWORDS: quantum computers, spin systems

## §1. Introduction

The idea that a Quantum Computer (QC) might be more powerful than an ordinary computer is based on the notion that a quantum system can be in any superposition of states and that interference of these states allows exponentially many computations to be done in parallel.[1)] A QC may solve certain computationally hard problems such as factoring integers and searching databases faster than a conventional computer.[2–7)] This intrinsic parallelism might be used to solve other difficult problems as well, such as for example the calculation of the physical properties of quantum many-body systems.[8–11)] In fact, part of Feynman's original motivation to consider QC's was that they might be used as a vehicle to perform exact simulations of quantum mechanical phenomena.[12)]

Theoretical work on quantum computation usually assumes the existence of units that perform highly idealized unitary operations. However, in practice these operations are difficult to realize. Disregarding decoherence, a hardware implementation of a QC will perform unitary operations that are more complicated than those considered in most theoretical work: In a QC the internal quantum dynamics of each elementary constituent is a key ingredient of the QC itself.

This paper describes a simulator for a generic physical model of a QC, strictly working according to the laws of quantum mechanics. We implement Grover's database search quantum algorithm (QA)[6,7)] using ideal and more realistic units, such as those used in the 2-qubit NMR QC.[13–17)]

* E-mail: deraedt@phys.rug.nl

## §2. Quantum Spin Dynamics

Generically, hardware QC's are modeled in terms of S=1/2 spins (qubits) that evolve in time according to the time-dependent Schrödinger equation (TDSE)

$$i\frac{\partial}{\partial t}|\Phi(t)\rangle = H(t)|\Phi(t)\rangle, \tag{2.1}$$

in units such that $\hbar = 1$ and where $|\Phi(t)\rangle$ describes the state of the whole QC at time $t$. The time-dependent Hamiltonian $H(t)$ takes the form

$$\begin{aligned} H(t) = &-\sum_{j,k=1}^{L}\sum_{\alpha=x,y,z} J_{j,k,\alpha}(t) S_j^\alpha S_k^\alpha \\ &-\sum_{j=1}^{L}\sum_{\alpha=x,y,z} \left(h_{j,\alpha,0}(t)\right. \\ &\left. +h_{j,\alpha,1}(t)\sin(f_{j,\alpha}t+\varphi_{j,\alpha})\right) S_j^\alpha, \end{aligned} \tag{2.2}$$

where the first sum runs over all pairs $P$ of spins, $S_j^\alpha$ denotes the $\alpha$-th component of the spin-1/2 operator representing the $j$-th qubit, $J_{j,k,\alpha}(t)$ determines the strength of the interaction between the qubits labeled $j$ and $k$, $h_{j,\alpha,0}(t)$ and $h_{j,\alpha,1}(t)$ are the static (magnetic) and periodic (RF) field acting on the $j$-th spin respectively. The frequency and phase of the periodic field are denoted by $f_{j,\alpha}$ and $\varphi_{j,\alpha}$. The number of qubits is $L$ and the dimension of the Hilbert space $D = 2^L$. Hamiltonian (2.2) captures the physics of most candidate technologies for building QC's.

A QA for the QC modeled by (2.1) and (2.2) consists of a sequence of elementary operations (EO's). The action of an EO on the state $|\Psi\rangle$ of the quantum processor is determined by the values of all the $J$'s and $h$'s (which are kept constant during the operation) and the time in-

terval it is active. The input state $|\Psi(t)\rangle$ is transformed into the output state $|\Psi(t+\tau)\rangle$ where $\tau$ denotes the time it takes to complete the EO. During this time interval the only time-dependence of $H(t)$ is through the (sinusoidal) modulation of the fields on the spins. The time evolution of the QC itself is governed by the TDSE (2.1).

Formally the solution of (2.1) can be expressed in terms of the unitary transformation $U(t+\tau,t) \equiv \exp_+(-i\int_t^{t+\tau} H(u)du)$, where $\exp_+$ denotes the time-ordered exponential function. Using the semi-group property of $U(t+\tau,t)$ we can write

$$U(t+\tau,t) = U(t+m\delta,t+(m-1)\delta)\cdots U(t+2\delta,t+\delta)U(t+\delta,t), \quad (2.3)$$

where $\tau = m\delta$ ($m \geq 1$). The standard procedure to construct algorithms for solving the TDSE (2.1) is to replace each $U(t+(n+1)\delta,t+n\delta)$ by a symmetrized product-formula approximation.[18–20] For the case at hand a convenient choice is (other decompositions[21,22] work equally well but are somewhat less efficient for our purposes):

$$U(t+(n+1)\delta,t+n\delta) \approx \widetilde{U}(t+(n+1)\delta,t+n\delta), \quad (2.4)$$

$$\begin{aligned}\widetilde{U}(t+(n+1)\delta,t+n\delta) = \\ e^{-i\delta H_z(t+(n+1/2)\delta)/2}e^{-i\delta H_y(t+(n+1/2)\delta)/2} \\ \times e^{-i\delta H_x(t+(n+1/2)\delta)}e^{-i\delta H_y(t+(n+1/2)\delta)/2} \\ \times e^{-i\delta H_z(t+(n+1/2)\delta)/2}, \end{aligned} \quad (2.5)$$

where

$$\begin{aligned}H_\alpha(t) = \\ -\sum_{j,k=1}^{L} J_{i,j,\alpha}S_j^\alpha S_k^\alpha \\ -\sum_{j=1}^{L}\left(h_{j,\alpha,0}+h_{j,\alpha,1}\sin(f_{j,\alpha}t+\varphi_{j,\alpha})\right)S_j^\alpha, \end{aligned} \quad (2.6)$$

with $\alpha = x,y,z$. In (2.6) the time dependence of the $J$'s and the $h$'s has been omitted because these parameters are constant during the execution of an EO.

Evidently $\widetilde{U}(t+\tau,t)$ is unitary by construction, implying that the algorithm to solve the TDSE is unconditionally stable.[18] It is easily shown that the algorithm is correct to second order in the time-step $\delta$.[18] Furthermore $\widetilde{U}(t+\tau,t)$ can be used as a building block to construct higher-order algorithms.[23–26] In practice it is easy to find reasonable, relatively small, values of $m$ such that the results obtained no longer depend on $m$ (and $\delta$). Then, for all practical purposes, these results are indistinguishable from the exact solution of the TDSE (2.1).

It is customary to take as basis states $\{|\phi_n\rangle\}$ the direct product of the eigenvectors of the $S_j^z$ (i.e. spin-up $|\uparrow\rangle_j$ and spin-down $|\downarrow\rangle_j$). In this basis $e^{-i\delta H_z(t+(n+1/2)\delta)/2}$ changes the input state by altering the phase of each of the basis vectors. As $H_z$ is a sum of pair interactions it is trivial to rewrite this operation as a direct product of 4x4 diagonal matrices (equivalent to the so-called interaction-controlled phase shifts) and 4x4 unit matrices. Hence the computation of $\exp(-i\delta H_z(t+(n+1/2)\delta)/2)|\Psi\rangle$ has been reduced to the multiplication of two vectors, element-by-element. The unitary matrix $e^{-i\delta H_y(t+(n+1/2)\delta)/2}$ can be written in a similar manner but the matrices that contain the interaction-controlled phase-shift have to be replaced by non-diagonal matrices. Although this does not present a real problem it is more efficient and systematic to proceed as follows. Let us denote by $\mathcal{X}$ ($\mathcal{Y}$) the rotation by $\pi/2$ of all spins about the $x(y)$-axis. As

$$\begin{aligned}e^{-i\delta H_y(t+(n+1/2)\delta)/2} &= \mathcal{X}\mathcal{X}^\dagger e^{-i\delta H_y(t+(n+1/2)\delta)/2}\mathcal{X}\mathcal{X}^\dagger \\ &= \mathcal{X}e^{-i\delta H'_z(t+(n+1/2)\delta)/2}\mathcal{X}^\dagger, \end{aligned} \quad (2.7)$$

it is clear that the action of $e^{-i\delta H_y(t+(n+1/2)\delta)/2}$ can be computed by applying to each qubit, the inverse of $\mathcal{X}$ followed by an interaction-controlled phase-shift and $\mathcal{X}$. The prime in (2.7) indicates that $J_{i,j,z}$, $h_{i,z,0}$, $h_{i,z,1}$ and $f_{i,z}$ in $H_z(t+(n+1/2)\delta)$ have to be replaced by $J_{i,j,y}$, $h_{i,y,0}$, $h_{i,y,1}$ and $f_{i,y}$ respectively. A similar procedure is used to compute the action of $e^{-i\delta H_x(t+(n+1/2)\delta)}$: We only have to replace $\mathcal{X}$ by $\mathcal{Y}$.

By construction our algorithm to solve the TDSE (2.1) for spin model (2.2) is a QA itself. As a real QC operates on all qubits simultaneously the operation counts for $e^{-i\delta H_x(t+(n+1/2)\delta)}$, $e^{-i\delta H_y(t+(n+1/2)\delta)/2}$, and $e^{-i\delta H_z(t+(n+1/2)\delta)/2}$ are $\mathcal{O}((P+2))$, $\mathcal{O}((P+2))$, and $\mathcal{O}(P)$.

## §3. Quantum Computation

Using the QA outlined above quantum spin systems containing up to 24 S=1/2 spins can easily be simulated on present-day supercomputers.[21] Here our aim is to use this QA to simulate a recent realization of a 2-qubit NMR QC[13,14,16,17] and to execute QA's on this simulator. In our calculations we will take the model parameters corresponding to the NMR experiments of Refs.16,17 in which the two nuclear spins of the $^1$H and $^{13}$C atoms in a carbon-13 labeled chloroform represent the two qubits.[16,17] In the NMR set-up the molecules are placed in a strong static magnetic field in the $+z$ direction. In the absence of interactions with other degrees of freedom this spin-1/2 system can be modeled by the hamiltonian

$$H = -J_{1,2,z}S_1^zS_2^z - h_{1,z,0}S_1^z - h_{2,z,0}S_2^z, \quad (3.1)$$

where $h_{1,z,0}/2\pi \approx 500$MHz, $h_{2,z,0}/2\pi \approx 125$MHz, and $J_{1,2,z}/2\pi \approx -215$Hz.[16] As the antiferromagnetic interaction between the spins is much weaker than the coupling to the external field and (3.1) is a diagonal matrix with respect to the basis states chosen, the ground state of (3.1) is the state with the two spins up ($|\uparrow\uparrow\rangle$). We denote this state by $|00\rangle = |\uparrow\rangle\otimes|\uparrow\rangle = |\uparrow\uparrow\rangle$, i.e. the state with spin up corresponds to a qubit $|\uparrow\rangle$. A state of the $N$-qubit QC will be denoted by $|x_1x_2\ldots x_N\rangle = |x_1\rangle\otimes|x_2\rangle\ldots|x_N\rangle$.

As usual it is expedient to write the TDSE for this NMR problem in frames of reference rotating with the nuclear spin. Substituting $|\Phi(t)\rangle =$

$e^{it(h_{1,z,0}S_1^z+h_{2,z,0}S_2^z)}|\Psi(t)\rangle$ the time evolution of $\Psi(t)$ in the absence of RF-fields is governed by the hamiltonian $H=-J_{1,2,z}S_1^zS_2^z$. This transformation has no effect on the expectation values of $z$-components of the spins but leads to oscillatory behavior of the $x$ or $y$ components, reflecting the fact that the spins are rotating about the $z$-axis. In the following it is implicitly assumed that the basis states of the spins refer to states in the corresponding rotating frame, even if we use the same notation for the basis states.

NMR uses radiofrequency electromagnetic pulses to rotate the spins.[27,28] By tuning the frequency of the RF-field to the precession frequency of a particular spin, the power (= intensity times duration) of the applied pulse controls how much the spin will rotate. The axis of the rotation is determined by the direction of the applied RF-field (see Refs. 27, 28).

## §4. Grover's database search algorithm

Finding a particular entry in an unsorted list of $N$ elements is a basic problem of searching databases. In general this takes of the order of $N$ operations on a conventional computer. It has been shown that a QC can find the item using only $\mathcal{O}\left(\sqrt{N}\right)$ attempts.[5,6]

Consider the extremely simple case of a database containing four items and functions $f_i(x)$ that upon query of the database return minus one for the particular item we are searching for and plus one otherwise. Assuming a uniform probability distribution for the item to be in one of the four locations, the average number of queries required by a conventional algorithm is 9/4. With Grover's QA the correct answer can be found in a single query (this result only holds for a database with 4 items). Grover's algorithm for the four-item database can be implemented on a 2-qubit QC.

The key ingredient of Grover's algorithm is an operation called "inversion about the mean" that replaces each amplitude of the basis states in the superposition by two times the average amplitude minus the amplitude itself. This allows then for the amplification of the amplitude of the basis state that represents the searched-for item. To see how this works it is useful to consider an example. Let us assume that the item to search for corresponds to e.g. number 2 ($f_2(0)=f_2(1)=f_2(3)=1$ and $f_2(2)=-1$). Using the binary representation of integers with the order of the bits reversed, the QC is in the state (up to an irrelevant phase factor as usual)

$$|\Psi\rangle=\frac{1}{2}(|\uparrow\uparrow\rangle+|\downarrow\uparrow\rangle-|\uparrow\downarrow\rangle+|\downarrow\downarrow\rangle). \tag{4.1}$$

We return to the question of how to prepare this state below. The operator $D$ that inverts states like (4.1) about their mean reads

$$D=\frac{1}{2}\begin{pmatrix}-1&1&1&1\\1&-1&1&1\\1&1&-1&1\\1&1&1&-1\end{pmatrix}\quad;\quad\begin{matrix}|\uparrow\uparrow\rangle\\|\downarrow\uparrow\rangle\\|\uparrow\downarrow\rangle\\|\downarrow\downarrow\rangle\end{matrix}. \tag{4.2}$$

The mean amplitude (i.e. the sum of all amplitudes divided by the number of amplitudes) of (4.1) is 1/4 and we find that

$$D|\Psi\rangle=|\uparrow\downarrow\rangle, \tag{4.3}$$

i.e. the correct answer, and

$$D^2|\Psi\rangle=\frac{1}{2}(|\uparrow\uparrow\rangle+|\downarrow\uparrow\rangle+|\uparrow\downarrow\rangle+|\downarrow\downarrow\rangle), \tag{4.4}$$

$$D^3|\Psi\rangle=-\frac{1}{2}(|\uparrow\uparrow\rangle+|\downarrow\uparrow\rangle-|\uparrow\downarrow\rangle+|\downarrow\downarrow\rangle)=-|\Psi\rangle, \tag{4.5}$$

showing that (in the case of 2 qubits) the correct answer (i.e. the absolute value of the amplitude of $|\downarrow\uparrow\rangle$ equal to one) is obtained after 1, 4, 7, ... iterations. In general, for more than two qubits, more than one application of $D$ is required to get the correct answer. In this sense the 2-qubit case is somewhat special.

The next task is to express the preparation and query steps in terms of elementary rotations. For illustrative purposes we stick to the example used above. We assume that initially the QC is in the state with both spins up ($|\uparrow\uparrow\rangle$). We follow the convention used earlier in this paper, i.e. the one used in Ref. 16) and therefore deviate from the notation used in Ref. 17). Transforming $|\uparrow\uparrow\rangle$ to the linear superposition (4.1) is a two-step process. First the QC is put into the uniform superposition state:

$$|U\rangle=W_2W_1|\uparrow\uparrow\rangle=-\frac{1}{2}(|\uparrow\uparrow\rangle+|\downarrow\uparrow\rangle+|\uparrow\downarrow\rangle+|\downarrow\downarrow\rangle), \tag{4.6}$$

where

$$W_j=X_jX_j\bar{Y}_j=-\bar{X}_j\bar{X}_j\bar{Y}_j=\frac{i}{\sqrt{2}}\begin{pmatrix}1&1\\1&-1\end{pmatrix}_j, \tag{4.7}$$

$$X_j\equiv e^{i\pi S_j^x/2\hbar}=\frac{1}{\sqrt{2}}\begin{pmatrix}1&i\\i&1\end{pmatrix}_j \tag{4.8}$$

and

$$\bar{Y}_j\equiv e^{-i\pi S_j^y/2\hbar}=\frac{1}{\sqrt{2}}\begin{pmatrix}1&-1\\1&1\end{pmatrix}_j \tag{4.9}$$

represents the Walsh-Hadamard (WH) transform on qubit $j$ which transforms $|\uparrow\rangle$ to $i(|\uparrow\rangle+|\downarrow\rangle)/\sqrt{2}$, a **clockwise** rotation of spin $j$ about $\pi/2$ around the $x$-axis and a **anti clock-wise** rotation of spin $j$ about $\pi/2$ around the $y$-axis respectively. The inverse of a rotation $Z$ is denoted by $\bar{Z}$. The second step is to encode the information in the database, e.g. $f_2(x)$, in the state of the QC. This can be accomplished by a transformation $F_i$ that in the case of our example $f_2(x)$ takes the form

$$F_2=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix}\quad;\quad\begin{matrix}|\uparrow\uparrow\rangle\\|\downarrow\uparrow\rangle\\|\uparrow\downarrow\rangle\\|\downarrow\downarrow\rangle\end{matrix}. \tag{4.10}$$

This transformation can be implemented by first letting the system evolve in time:

$$\begin{aligned}I(\pi)|U\rangle&=e^{-i\pi S_1^zS_2^z}\left[\frac{1}{2}(|\uparrow\uparrow\rangle+|\downarrow\uparrow\rangle+|\uparrow\downarrow\rangle+|\downarrow\downarrow\rangle)\right]\\&=\frac{1}{2}(e^{-i\pi/4}|\uparrow\uparrow\rangle+e^{+i\pi/4}|\downarrow\uparrow\rangle\\&\quad+e^{+i\pi/4}|\uparrow\downarrow\rangle+e^{-i\pi/4}|\downarrow\downarrow\rangle).\end{aligned} \tag{4.11}$$

For the NMR-QC based on hamiltonian (3.1) this means letting the system evolve in time (without applying pulses) for a time $\tau_0 = -\pi/J_{1,2,z}$ (recall $J_{1,2,z} < 0$).

Next we apply a sequence of single-spin rotations to change the four phase factors such that we get the desired state. The two sequences $YX\bar{Y}$ and $Y\bar{X}\bar{Y}$ are particulary useful for this purpose. We find

$$\begin{aligned} Y_1X_1\bar{Y}_1Y_2\bar{X}_2\bar{Y}_2 &\left[\frac{1}{2}(e^{-i\pi/4}|\uparrow\uparrow\rangle + e^{+i\pi/4}|\downarrow\uparrow\rangle\right. \\ &\left.+e^{+i\pi/4}|\uparrow\downarrow\rangle + e^{-i\pi/4}|\downarrow\downarrow\rangle)\right] \\ &= \frac{1}{2}(e^{-i\pi/4}|\uparrow\uparrow\rangle + e^{-i\pi/4}|\downarrow\uparrow\rangle \\ &+e^{+3i\pi/4}|\uparrow\downarrow\rangle + e^{-i\pi/4}|\downarrow\downarrow\rangle) \\ &= \frac{e^{-i\pi/4}}{2}(|\uparrow\uparrow\rangle + |\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle + |\downarrow\downarrow\rangle). \end{aligned} \quad (4.12)$$

Combining (4.11) and (4.12) we can construct the sequence transforming the uniform superposition in the state that corresponds to $f_i(x)$:

$$F_0 = Y_1\bar{X}_1\bar{Y}_1Y_2\bar{X}_2\bar{Y}_2I(\pi), \quad (4.13a)$$

$$F_1 = Y_1\bar{X}_1\bar{Y}_1Y_2X_2\bar{Y}_2I(\pi), \quad (4.13b)$$

$$F_2 = Y_1X_1\bar{Y}_1Y_2\bar{X}_2\bar{Y}_2I(\pi), \quad (4.13c)$$

$$F_3 = Y_1X_1\bar{Y}_1Y_2X_2\bar{Y}_2I(\pi). \quad (4.13d)$$

The remaining task is to express the process of inversion about the mean, i.e. the matrix $D$ (see (4.2)), by a sequence of elementary operations. It is not difficult to see that $D$ can be written as the product of a WH transform, a conditional phase shift $P$ and another WH transform:

$$\begin{aligned} D &= W_1W_2PW_1W_2 \\ &= W_1W_2\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}W_1W_2. \end{aligned} \quad (4.14)$$

The same approach that was used to implement $f_2(x)$ also works for the conditional phase shift $P$ ($= -F_0$) and yields

$$P = Y_1\bar{X}_1\bar{Y}_1Y_2\bar{X}_2\bar{Y}_2I(\pi). \quad (4.15)$$

The complete sequence $U_i$ reads

$$U_i = W_1W_2PW_1W_2F_i. \quad (4.16)$$

Each sequence $U_i$ can be shortened by observing that in some cases a rotation is followed by its inverse. As there are various representations of the WH transform $W_i$ that accomplish the same task, the sequence for e.g. $i = 2$ can be written as

$$\begin{aligned} W_1W_2F_2 &= -\bar{X}_1\bar{X}_1\bar{Y}_1X_2X_2\bar{Y}_2Y_1X_1\bar{Y}_1Y_2\bar{X}_2\bar{Y}_2I(\pi) \\ &= -\bar{X}_1\bar{Y}_1X_2\bar{Y}_2I(\pi). \end{aligned} \quad (4.17)$$

The sequences for the other cases can be shortened as well, yielding

$$U_0 = X_1\bar{Y}_1X_2\bar{Y}_2I(\pi)X_1\bar{Y}_1X_2\bar{Y}_2I(\pi), \quad (4.18a)$$

$$U_1 = X_1\bar{Y}_1X_2\bar{Y}_2I(\pi)X_1\bar{Y}_1\bar{X}_2\bar{Y}_2I(\pi), \quad (4.18b)$$

$$U_2 = X_1\bar{Y}_1X_2\bar{Y}_2I(\pi)\bar{X}_1\bar{Y}_1X_2\bar{Y}_2I(\pi), \quad (4.18c)$$

$$U_3 = X_1\bar{Y}_1X_2\bar{Y}_2I(\pi)\bar{X}_1\bar{Y}_1\bar{X}_2\bar{Y}_2I(\pi), \quad (4.18d)$$

where in $U_1$ and $U_2$ we have dropped a physically irrelevant sign. Note that the binary representation of $i$ translates into the presence (1) or absence (0) in (4.18) of a bar on the rightmost $X_1$ and $X_2$.

Table I. Specification of the EO's of a mathematically perfect 2-qubit QC. The execution time of each micro instruction is given by the second row ($\tau/2\pi$). The inverse of e.g. $\bar{X}_1$ is found by reversing the sign of $h_{1,x,0}$. Model parameters omitted are zero for all EO's.

| | $X_1$ | $\bar{X}_2$ | $Y_1$ | $\bar{Y}_2$ | $I(\pi)$ |
|---|---|---|---|---|---|
| $\tau/2\pi$ | 0.25 | 0.25 | 0.25 | 0.25 | $50 \times 10^4$ |
| $J_{1,2,z}$ | 0 | 0 | 0 | 0 | $-10^{-6}$ |
| $h_{1,x,0}$ | +1 | 0 | 0 | 0 | 0 |
| $h_{2,x,0}$ | 0 | −1 | 0 | 0 | 0 |
| $h_{1,y,0}$ | 0 | 0 | +1 | 0 | 0 |
| $h_{2,y,0}$ | 0 | 0 | 0 | −1 | 0 |

Table III. Final state of the qubits after running the Grover's database search algorithm on an ideal QC ($Q_1, Q_2$, model parameters given in table I), on a NMR-QC ($\hat{Q}_1, \hat{Q}_2$, model parameters given in table II) and on the same NMR-QC ($\tilde{Q}_1, \tilde{Q}_2$, model parameters given in table II) using a different, but logically equivalent, initialization sequence.

| | $U_0\|U\rangle$ | $U_1\|U\rangle$ | $U_2\|U\rangle$ | $U_3\|U\rangle$ |
|---|---|---|---|---|
| $Q_1$ | 0.000 | 1.000 | 0.000 | 1.000 |
| $Q_2$ | 0.000 | 0.000 | 1.000 | 1.000 |
| $\hat{Q}_1$ | 0.028 | 0.966 | 0.037 | 0.955 |
| $\hat{Q}_2$ | 0.163 | 0.171 | 0.836 | 0.830 |
| $\tilde{Q}_1$ | 0.955 | 0.041 | 0.971 | 0.027 |
| $\tilde{Q}_2$ | 0.031 | 0.026 | 0.971 | 0.972 |

## §5. Results

We now consider two different implementations of the Grover's QA described above. The first and most obvious one is to make use of theoretically ideal unitary transformations to perform the EO's. One of the many possible choices for the model parameters that correspond to this case are given in Table I. The second will be physical, i.e. we will use the simulator to carry out the NMR-QC experiment itself. The list of model parameters can be found in Table II. The values of the qubits $(Q_1, Q_2)$ are given by

$$Q_i \equiv \frac{1}{2} - \langle S_i^z \rangle, \quad (5.1)$$

The numerical values of the qubits in the final state as obtained by running Grover's QA on the simulator are summarized in Table III. From the data in the first two rows it is evident that this QA performs as expected when the ideal EO's are used. In the ideal case, the final state $(Q_1, Q_2)$ is the binary representation of the integer index of the "-1" item.

Table II. Specification of the elementary operations implementing a 2-qubit NMR QC, using the notation of Table 1. Note that a RF-pulse along the $y(x)$ direction corresponds to a rotation about the $x(y)$. Model parameters omitted are zero for all EO's.

| | $X_1$ | $\bar{X}_2$ | $Y_1$ | $\bar{Y}_2$ | $I(\pi)$ |
|---|---|---|---|---|---|
| $\tau/2\pi$ | 10 | 40 | 10 | 40 | $50 \times 10^4$ |
| $J_{1,2,z}$ | $-10^{-6}$ | $-10^{-6}$ | $-10^{-6}$ | $-10^{-6}$ | $-10^{-6}$ |
| $h_{1,z,0}$ | 1 | 1 | 1 | 1 | 1 |
| $h_{2,z,0}$ | 0.25 | 0.25 | 0.25 | 0.25 | 0.25 |
| $h_{1,x,1}$ | 0 | 0 | 0.05 | $-0.05$ | 0 |
| $h_{2,x,1}$ | 0 | 0 | 0.0125 | $-0.0125$ | 0 |
| $f_{1,x}$ | 0 | 0 | 1 | 0.25 | 0 |
| $f_{2,x}$ | 0 | 0 | 1 | 0.25 | 0 |
| $h_{1,y,1}$ | $-0.05$ | 0.05 | 0 | 0 | 0 |
| $h_{2,y,1}$ | $-0.0125$ | 0.0125 | 0 | 0 | 0 |
| $f_{1,y}$ | 1 | 0.25 | 0 | 0 | 0 |
| $f_{2,y}$ | 1 | 0.25 | 0 | 0 | 0 |

The third and fourth row contain the data for the NMR-QC case. Using RF-pulses instead of ideal transformations to perform $\pi/2$ rotations leads to less certain answers: The final state is no longer a pure basis state but some linear superposition of the four basis states. Indeed, using a time-dependent external pulse to rotate spins only yields an approximation to the simple rotations envisaged in theoretical work. This affects the expectation values of the spin operators. What is beyond doubt though is that it is easy to read off the correct answer from the expectation values of the qubits. Clearly the simulator reproduces the experimental results and the QA seems to return the correct answer.

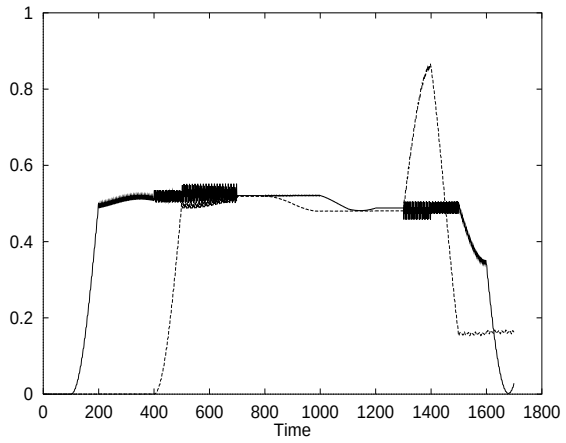


Fig. 1. Time evolution of the qubits $Q_1$ (solid line) and $Q_2$ (dashed line) obtained by executing $W_1$, $W_2$ and sequence (4.18a) for the case of the NMR-QC. In all figures the time intervals for each operation have been rescaled to make them look equal.

In an NMR experiment, application of each RF-pulse affects all spins in the sample. Although the response of a spin to the RF-field will only be large when this spin is at resonance, the state of the spins that are not in resonance will also change. These successive unitary transformations not necessarily commute with each other. If they do not commute the state after these transformations depends on the order in which the pulses have been applied. In fact the presence of these perturbations, although small, can have a devastating effect on the stability of the computation. This is illustrated by the data in the fifth and sixth row of Table III and by Figs. 1- 4. These results have been obtained by changing the order of preparing the two spin states. Instead of $W_1W_2$ we used $W_2W_1$ to initialize the QC, a permutation that has no effect in the case of ideal EO's. From Table III it is clear that in the case of EO's implementing the 2-qubit NMR QC making this interchange leads to complete wrong results. Many of such examples can be

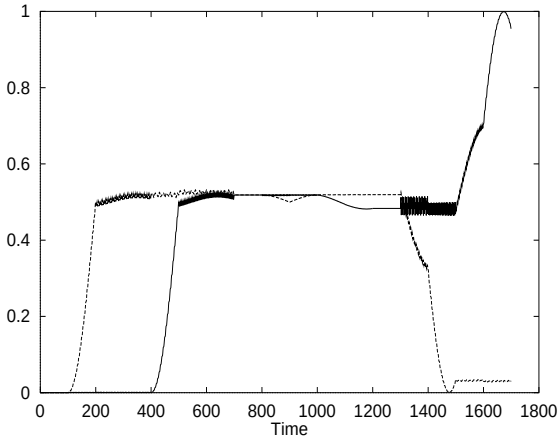


Fig. 2. Time evolution of the qubits $\tilde{Q}_1$ (solid line) and $\tilde{Q}_2$ (dashed line) obtained by executing $W_2$, $W_1$ and sequence (4.18a) for the case of the NMR-QC. Interchanging the order in which the single-qubit operations $W_1$ and $W_2$ are applied changes the final state of the QC.

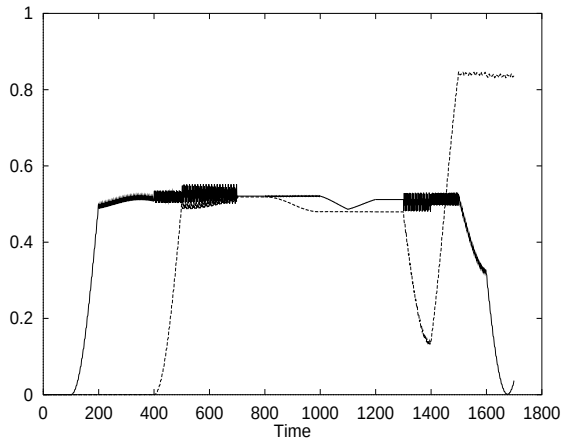


Fig. 3. Same as Fig.1 but instead of sequence (4.18a) we used (4.18c).

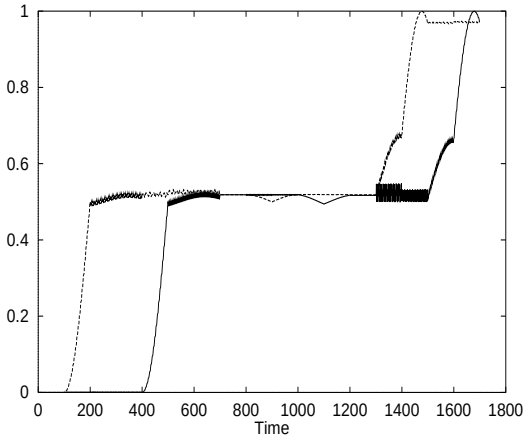


Fig. 4. Same as Fig.2 but instead of sequence (4.18a) we used (4.18c).

constructed: The very fact that we cannot isolate one spin from the rest and perform operations on the former only leads to phase errors that may (but sometimes don't) alter the outcome of the calculation completely. This QC architecture is intrinsically unstable to minor modifications of the QA that are allowed from logical point of view, a much more severe problem than that of "decoherence". We believe it might be interesting to investigate these instabilities experimentally.

Can the phase errors discussed above be (partially) eliminated by some clever error-correction scheme? At present there is no indication they can: Any error-correction method requires adding extra spins to the system. The phase shift incured by the individual spins will contribute to the phase shifts of each of the many-body basis states and unless some magic cancelation takes place, the final result is unlikely to be more stable. On the other hand these unwanted phase factors are the result of using RF pulses that only approximately implement rotations about 90 degrees and may be reduced by using pulses that are more complicated than the sinusoidal ones. Perhaps dissipation effects may also help to reduce the sensitivity to phase errors, a possibility that we are currently investigating. Another route to more stable operation might be to use a different set of EO's that more closely implements the ideal transformations. For instance, non-adiabatic transitions between two levels driven by a periodic field display peculiar behavior[29] and might be employed to manipulate the two-level systems. In this respect the single-Cooper-pair-box[30] may hold some promise. In this solid-state device a non-adiabatic transition mechanism is used to let a Cooper pair tunnel between two states. Obviously there are many physical mechanisms to control the dynamics of quantum spin systems. Exploring which of these mechanisms is useful for quantum computing may be a fertile area for future research.

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