Simulation of Grover’s quantum search algorithm in an Ising-nuclear-spin-chain quantum computer with first- and second-nearest-neighbour couplings

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Abstract

We implement Grover’s quantum search algorithm on a nuclear spin-chain quantum computer, taking Ising-type interactions between nearest and second-nearest neighbours into account. The performance of this implementation is studied by numerical simulations with four spins. We determine the temporal behaviour of the fidelity during the algorithm, and we compute the final fidelity as a function of the Rabi frequency. For the latter, we obtain pronounced maxima at frequencies which fulfil the condition of the \(2\pi k\)-method with respect to the second-nearest-neighbour interactions.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The Ising-spin-chain quantum computer is a simple theoretical model system, which has many of the relevant features of a physical realization of a quantum computer. The bare model is defined in terms of a time-independent Hamiltonian \(H_0\), describing a system of spins in a strong magnetic field and coupled by the Ising interaction. Additional time-dependent perturbations (e.g. radio-frequency pulses, which may be switched on and off at will) are used to implement certain elementary quantum gates, from which any unitary quantum algorithm can be constructed (universal quantum gates).

Originally, this model has been proposed in [1–4], and a large number of theoretical studies has been devoted to it (to mention a few important works [5–7]). As a physical realization, one may think of nuclear spins embedded in a solid state system in an external strongly inhomogeneous magnetic field. Ultracold atoms in optical lattices provide a possibly less demanding alternative [8].

In this case, the bare Hamiltonian becomes

\[
\frac{1}{\hbar} H_0 = -\sum_{k=1}^{n} w_k I_z^k - 2J \sum_{k=1}^{n-1} I_z^k I_z^{k+1} - 2J' \sum_{k=1}^{n-2} I_z^k I_z^{k+2},
\]

where \(w_k\) is the Larmor frequency of spin \(k\). Since the dipole interactions may be induced by electron clouds around the nuclear spins, it is realistic to consider \(J\) and \(J'\) as independent parameters. The Hamiltonian \(H_0\) is diagonal in the so-called computational basis, which consists of products of single spin (qubit) eigenstates of \(I_z\), which are denoted by \(|0_k\rangle\) and \(|1_k\rangle\), respectively,

\[
I_z^k |\alpha_k\rangle = (-1)^{\alpha_k} \frac{1}{2} |\alpha_k\rangle.
\]

In order to implement the desired quantum gates, we use monochromatic electromagnetic radio-frequency pulses (RF-pulses) described by the term \(W(t)\),

\[
H = H_0 + W(t),
\]

\[
W(t) = \frac{\hbar \Omega}{2} \sum_{k=0}^{n-1} \left( e^{i(\omega_k t)} I_z^k + e^{-i(\omega_k t)} I_z^k \right),
\]

In the present work, we assume an Ising interaction between nearest and next-nearest (second) neighbours [9, 10].
where the frequency \( w \), the phase offset \( \varphi \) and the Rabi frequency \( \Omega \) are free parameters (\( \Omega / \gamma \) is the amplitude of the electromagnetic field and \( \gamma \) is the gyromagnetic ratio for the spins). \( H^k = (I^k)^\dagger = |0_k\rangle\langle 1_k| \) is the raising operator of qubit \( k \). The desired quantum gates (and the whole quantum algorithm) are realized within the interaction picture. We apply the above-defined RF-pulses with a rectangular envelope, choosing the frequency \( w \) in resonance with an appropriate transition in \( H_0 \). The resulting unitary evolution is denoted by

\[
R^k_{\mu}(\varphi, \vartheta) \quad w = w_k + \mu J + v J',
\]

(4)

where \( \mu \) and \( v \) are integers. The angle \( \varphi \) gives the phase offset of the RF-pulse, whereas \( \vartheta = \Omega \tau \) determines the duration \( \tau \) of the pulse. The RF-pulses are selected in such a way that they yield the desired quantum gates exactly, if all off-resonant transitions are neglected (resonant approximation). The 'real' evolution will be obtained from numerical simulations, where all transitions are taken into account. The deviation from the 'ideal' evolution is quantified by fidelity [11], the absolute value squared of the wavefunction overlap for both evolutions.

In order to minimize the decay of fidelity, we apply the \( 2nR \)-method to suppress those transitions which are nearest to resonance, which in our case are related to the second-neighbour interaction [10]. The resulting condition for the Rabi frequency reads

\[
\Omega = \Omega^{(e)} = \frac{2J'}{\sqrt{4k^2-1}}.
\]

(5)

In the present work, we study the effects of unitary errors (due to non-resonant transitions) on a quantum algorithm of intermediate length. Such an algorithm may consist of several hundreds of pulses, even though it is still far away from the regime, where a quantum computer could really demonstrate its superiority over a classical one (after all, our work rely on numerical simulations on a classical PC). It is however also far beyond pulse sequences, which only realize one or a few elementary qubit gates. Of particular interest will be the question whether we can from the fidelity decay of few gate operations extrapolate to the fidelity decay of the whole quantum algorithm.

As an example we consider Grover's quantum search algorithm [12, 13]. This algorithm is one of the two prime examples where a quantum computer is superior to any classical computer. It finds a marked item in an unsorted data base with a quadratic speed-up over any classical search algorithm. Recent work has been focused on experimental realizations [14, 15]—still limited to a very small data register of only two qubits, on proposals for experimental realizations with larger data registers [16–18], and on theoretical studies of the stability of Grover's algorithm [19–21]. Our implementation follows closely the presentation in [22]. Its basic elements are single-qubit Hadamard gates. Due to the Ising interactions, these gates are quite expensive in the Ising-spin-chain quantum computer as we will see below. The big majority of the pulses are used to implement these gates. The other gates are \( n \)-qubit phase gates, where \( n \) is the number of bits of the search space. In our case we use a spin chain of length 4, where one of the spins serves as the ‘ancilla’ qubit, such that \( n = 3 \). Note, that there exists an improved version [23], which corrects the relatively high failure rate for small state spaces (as the one used here). We have checked that the improved algorithm of [23] leads to very similar results; see the discussion in the conclusions, section 4.

In the following section (section 2), we will discuss Grover’s search algorithm as such, and its implementation in the Ising-spin-chain quantum computer. In section 3, we show numerical simulations of the search algorithm, discuss the fidelity decay during the execution of the algorithm, and study the final fidelity as a function of the Rabi frequency. Conclusions are provided in section 4.

2. Realization of Grover’s search algorithm

In its most basic form [22], Grover’s quantum search algorithm requires \( n \) qubits to prepare the ‘enquiry’ states (in the data register) subsequently presented to the ‘oracle’, and a single additional qubit (the ‘ancilla’ qubit) used by the oracle to ‘communicate’ its answer. The algorithm starts with the data register in the ground state, \( \{0_n\} \), and in an initial step, Hadamard gates are applied to all qubits, thereby leaving the data register in the total superposition of all basis states. This sequence of Hadamard gates will be denoted by \( H^{\otimes n} \). The creation of the superposition state is followed by a Grover operator, which may be repeated several times, until the data register contains the desired target state with sufficiently high probability. The Grover operator is again composed of Hadamard gates and conditional phase reflections,

\[
G = O(\alpha)H^{\otimes n}S_0H^{\otimes n}.
\]

(6)

where \( \alpha \) may be any number representable in the data register. The unitary oracle \( O(\alpha) \), leaves all basis states untouched, except for the state \( |\alpha\rangle \), to which it applies a sign change (phase reflection). The other unitary operator \( S_0 \), in turn, changes the sign of all basis states but leaves the state \( |0\rangle \) untouched. While the Hadamard gates are single qubit gates, \( O(\alpha) \) and \( S_0 \) are true \( (n+1)\)-qubit gates.

In this work, we implement the Grover algorithm in a quantum register of four qubits \( |i_1, i_2, i_3, i_4\rangle \). For numerical simulations, it is convenient to use the qubits \( k = 0, 2, 3 \) as data register, and the qubit \( k = 1 \) as the ancilla qubit. In this way, the ancilla qubit is coupled directly (by first- or second-neighbour couplings) to all qubits in the data register. In what follows, we discuss the implementation of the Hadamard gates, the conditional phase reflection \( S_0 \) and the oracle in separate subsections.

2.1. Hadamard gates

The Hadamard gate is a single qubit gate. In the Hilbert space of that qubit the gate acts as a unitary matrix,

\[
H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.
\]

(7)

It can be decomposed into elementary qubit rotations as follows:

\[
H = R_y(\tau)R_x(\tau/2)R_y(\tau),
\]

(8)
where \( R_0(\theta) = R(\pi/2, \theta) \) and
\[
R(\varphi, \theta) = \begin{pmatrix}
\cos(\varphi/2) & i e^{i \varphi} \sin(\varphi/2) \\
i e^{-i \varphi} \sin(\varphi/2) & \cos(\varphi/2)
\end{pmatrix}.
\] (9)

The single qubit rotations of the form (9) may be obtained by applying appropriate electromagnetic pulses as defined in (3) and (4) to the Ising spin chain. In the presence of neighbouring qubits, one has to repeat that pulse sequence for all possible configurations of the neighbouring qubits, in order to obtain the true single qubit gate, independent of the state of the data register.

Formally, the gate \( S \) may be implemented by a single 2-pulse sequence:
\[
S(\alpha) = (-1 + 2 \delta_{\alpha,0}) \alpha.
\] (10)

The overall error can be further decreased by rearrangements for \( H_5 \) and \( H_1 \).

The overall error can be further decreased by rearranging the outer sequences of \( \pi \)-pulses in a similar manner into sequences of single qubit \( \pi/2 \)-pulses. These measures drastically increase the number of pulses for the implementation of the algorithm. Now, we need 20 pulses for the \( H_0 \) and \( H_3 \) gates and 30 pulses for the \( H_2 \) gate. In total this gives 70 pulses for the \( H^{\otimes 3} \) gate and 146 pulses for each Grover operator step. Note however that the amount of time to implement those gates is the same as before.

In this section, we are mainly concerned with unitary errors due to non-resonant transitions, and due to phase errors which are not suppressed by the \( 2\pi k \)-method. Thus, we will study in some detail the behaviour of fidelity [11] during the algorithm. The fidelity, \( f(t) \), is the overlap between the state evolving under the ideal evolution (where only resonant transitions are taken into account) and the state evolving under the true evolution governed by the Hamiltonian in equation (3). The fidelity (or fidelity amplitude) is a complex quantity, and we will normally study its absolute value squared, \( |f(t)|^2 \). In the simulations described below, the Larmor frequencies are chosen as \( \omega_0 = 100, \omega_1 = 200, \omega_2 = 400 \) and \( \omega_3 = 800 \). The nearest- and next-nearest-neighbour coupling parameters are fixed to \( J = 10 \) and \( J' = 0.4 \) (with the exception of figure 5, where \( J' \) is varied).
Figure 1. The absolute value squared of the fidelity during the Grover algorithm with two Grover operator steps. Time is measured in units of the duration of a single $\pi/2$-pulse. The algorithm is simulated for different target states $|\alpha\rangle$ (see legend). The Rabi frequency is $\Omega = 0.108$, which suppresses non-resonant transitions as far as possible.

Figure 2. The absolute value squared of the fidelity during the Grover algorithm with two Grover operator steps. Time is measured in units of the duration of a single $\pi/2$-pulse. The algorithm is simulated for different target states $|\alpha\rangle$ (see legend). The Rabi frequency is $\Omega = 0.135$, which yields similarly high fidelities as in figure 1. The smooth blue line shows an exponential, fitted to the initial preparation step ($t/\tau_{\pi/2} < 70$). The fastest decay, roughly following the exponential is obtained for random initial states (lowest red curve). Otherwise, the Rabi frequency is fixed to $\Omega = 0.108$ which approximately fulfils the $2\pi k$-condition (5) with $k = 4$. The same set of parameters has been used in [9, 10].

Figure 1 shows $|f(t)|^2$ during the whole search algorithm for four different target states, selected by different oracle pulses: red curve ($\alpha = 0$), blue curve ($\alpha = 5$), light blue curve ($\alpha = 8$) and pink curve ($\alpha = 13$). As mentioned above, the Rabi frequency fulfils the $2\pi k$-condition (5) with $k = 4$. Since $k$ is even, non-resonant transitions are suppressed during $\pi$-pulses, as well as $\pi/2$-pulses; see [10].

Figure 2 shows $|f(t)|^2$ for the same Grover algorithm, but for the Rabi frequency, $\Omega = 0.135$, which is close to $\Omega^{(3)}$ as given by the $2\pi k$-condition (5). Since $k$ is odd in this case, one would expect that non-resonant transitions were suppressed during $\pi$-pulses, but not during $\pi/2$-pulses. Still, we find similarly high fidelities as in the previous case. This surprising result is discussed in more detail, below. In this figure, the fidelity along the full algorithm does not follow the initial trend of relatively fast decay. To obtain that initial trend, we fitted an exponential to the initial preparation step (the first 70 $\pi/2$-pulses). This non-generic behaviour is interesting, because it shows that it is not sufficient to characterize the performance of individual quantum gates by their average fidelity-loss rates. With no other information than such loss rates, one would greatly underestimate the overall fidelity of the algorithm. A convenient way to obtain average loss rates is to use random initial states. The lower red curve shows $|f(t)|^2$ averaged over 100 different initial states chosen at random from the invariant (under unitary transformations) ensemble of normalized states. The curve still shows large fluctuations which should disappear in the limit of a larger sample size. However, the general trend of a global exponential decay is clearly observable. It also agrees quite nicely with the exponential fit (smooth blue curve).

In figure 3, the Rabi frequency is chosen to allow non-resonant transitions ($\Omega = 0.2550$). By consequence, we find...
we should expect rather small fidelities at Rabi frequencies \( \pi/\Omega \) odd values of \( \pi/k \). For \( \pi/k \)-transitions only for the coupling parameter. In this case, the Rabi frequency was near \( \pi/k \). The Rabi frequency obtained from equation (5) selects the target state of the Rabi frequency. We chose the oracle whole algorithm with two Grover operator steps as a function of \( J' \), the next-nearest-neighbour coupling parameter. In that case, the maxima of the final fidelity remain close to one, whether the \( 2\pi k \)-condition is fulfilled or not. The reason is that the frequency mismatch of the non-resonant transitions becomes so large, that they are ever more unlikely to occur.

This changes only when \( J' \) gets close to \( J \), such that non-resonant transitions with detunings of the order of \( |J' - J| \) become relevant. This regime is shown in figure 5(b), where the final fidelity is plotted versus the difference between the parameters for the second- and first-nearest-neighbour couplings. In that case, the maxima of the final fidelity are approximately given by the \( 2\pi k \)-condition applied to that new scale \( |J' - J| = \sqrt{4k^2 - 1}/\Omega/2 \). The vertical lines show the precise values of \( J' - J \) for \( k = 1, \ldots, 3 \). The Rabi frequency \( \Omega = 0.2582 \) was chosen such that the \( 2\pi k \)-condition was approximately fulfilled at \( |J' - J| = 1 \) (for \( k = 2 \)).

In the case of figure 5(a), we also performed simulations, where we adjusted \( \Omega \) to the changing coupling parameter \( J' \) such that the \( 2\pi k \)-condition was fulfilled for any value of \( J' \). In that case the final fidelity remained close to one over the whole range of values. However, this meant that we had to decrease \( \Omega \) proportional to \( J' \), which lead to an inversely proportional increase of the duration of the whole algorithm. This is for many reasons (e.g. decoherence) impractical.

4. Conclusions

We implemented Grover’s quantum search algorithm on an Ising spin chain of length 4, taking into account first and second neighbour couplings. The coupling strength of second neighbours is much weaker than that of first neighbours, which means that the dominant source for errors are near-resonant transitions, where the detuning is of the order of \( J' \). In other words, the second neighbour couplings are the dominant source for errors in our setup. The accumulated errors in the course of the quantum algorithm are quantified by the fidelity. We investigated its temporal behaviour as well as its final value, as a function of the Rabi frequency and the coupling parameter \( J' \).
We used the $2\pi k$-method to suppress non-resonant transitions. Since the great majority of the RF-pulses used are $\pi/2$-pulses, we would have expected high fidelities at Rabi frequencies corresponding to even $k$, but rather low fidelities for odd $k$. Surprisingly, however, we found similarly pronounced maxima in both cases. In addition, we found that by properly rearranging the RF-pulses, the errors in the implementation of the Hadamard gates are greatly reduced. By properly choosing the Rabi frequency we obtained fidelities beyond 90%, for the whole algorithm with two Grover steps. This corresponds to an average loss of fidelity of the order of $4 \times 10^{-4}$ (per $\pi$-pulse) and $6 \times 10^{-3}$ (per Hadamard gate), numbers which are compatible with recent requirements for fault tolerant quantum computation [24].

However, we also found a strongly fluctuating fidelity decay with eventual revivals on time scales which correspond approximately to the duration of a Grover step. This complicated picture was roughly the same, no matter whether the non-resonant transitions have been strongly suppressed (figure 1 and 2) or not (figure 3). This shows that a simple error model which assigns state-independent failure rates to the different quantum gates, may not be appropriate.

An optimized algorithm, with zero failure rate (error-free case), has been developed in [23]. With that modification and taking only resonant transitions into account, our algorithm with two Grover steps indeed succeeds in finding the target state with 100% probability. We performed simulations with the modified algorithm, similar to those, which lead to the figures 1–3. We found that the fidelity decay induced by the non-resonant transitions is qualitatively similar, and leads to final fidelities of approximately the same magnitude.

A general scheme for the analysis of decoherence in large quantum registers under local dynamics has been put forward in [25]. On the one hand, we may generalize this scheme to include unitary errors. This might offer a viable method to describe the complicated relative dynamics (relative to the ideal evolution) observed in this work. On the other hand, we also performed some preliminary studies using fluctuating Larmor frequencies (simulating tiny variations of the external magnetic field). This is a simple way to introduce decoherence into our model. As a result, we could apply the scheme proposed in [25] to describe the decoherence in the initial step of the Grover algorithm, since that part contains only local operations.

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