Complexity of decoupling and time-reversal for $n$ spins with pair-interactions: 
Arrow of time in quantum control

Dominik Janzing*, Pawel Wocjan, and Thomas Beth
Institut für Algorithmen und Kognitive Systeme, Am Fasanengarten 5, D–76 131 Karlsruhe, Germany

Well-known Nuclear Magnetic Resonance experiments show that the time evolution according to (truncated) dipole-dipole interactions between $n$ spins can be inverted by simple pulse sequences. Independent of $n$, the reversed evolution is only two times slower than the original one. Here we consider more general spin-spin couplings with long range. We prove that some are considerably more complex to invert since the number of required time steps and the slow-down of the reversed evolutions are necessarily of the order $n$. Furthermore, the spins have to be addressed separately. We show for which values of the coupling parameters the phase transition between simple and complex time-reversal schemes occurs.

Due to wide applications of Nuclear Magnetic Resonance in medicine, chemistry, and physics much effort has been undertaken to understand the dynamics of nuclear spins in solids and liquids \cite{4,6,5,7}. Nowadays, NMR plays an important role in the first experimental realizations of quantum computation \cite{1,2}

Phenomenologically, the dynamical evolution of a single spin seems to be a relatively simple relaxation and dephasing process of an open quantum system, formally described by the Bloch equations \cite{3,4}. However, the fact that not all dephasing and relaxation processes are irreversible is important for practical purposes since refocusing techniques are applied with great success \cite{4,6,5,7}.

The simplest version of refocusing is possible when dephasing of the (uncoupled) spins is caused by spatial inhomogeneities of the strength of the magnetic field. In this case the time evolution can be reversed by sandwiching the natural dynamics by 180°-rotations of all spins around an axis orthogonal to the magnetic field. More sophisticated versions of refocusing are necessary if dephasing and relaxation processes are caused by spin-spin interactions. An important example is the so-called dipole-dipole coupling \cite{3,4}.

We describe this interaction formally as follows. Let $(\mathbb{C}^2)^\otimes n$ be the Hilbert space of $n$ spins and $\rlap.{\sigma}^k_{\alpha}$ be the Pauli matrix $\sigma_{\alpha}$ acting on the $k$-th spin for $1 \leq k \leq n$ and $\alpha = x, y, z$. Then the so-called truncated dipole-dipole Hamiltonian $H_d$ is given by

$$H_d := \sum_{k < l} w_{kl} \left( \sum_{\alpha} \sigma_{\alpha}^{(k)} \sigma_{\alpha}^{(l)} - 3 \sigma_{z}^{(k)} \sigma_{z}^{(l)} \right),$$

where $w_{kl}$ is the strength of the interaction between the spins $k$ and $l$.

We assume that all local unitary operations on the spins can be produced in arbitrarily small time (on a time scale governed by the strength of the coupling). This is often called the fast control limit. In practice this is done by external electro-magnetic pulses.

Consider a pulse implementing a rotation of each spin around the $y$-axis by 90°, i.e., if the spin is in $z$-direction it is in $x$-direction after the rotation. Formally, one applies a unitary transformation on $(\mathbb{C}^2)^\otimes n$ of the form

$$v_y := u_y \otimes u_y \otimes \cdots \otimes u_y$$

with $u_y \sigma_z u_y = \sigma_x$. Now we focus on the effect of the following scheme: (1) implement $v_y$ by the corresponding pulse, (2) wait the time $t$, and (3) implement $v_y^\dagger$, i.e., the inverse of $v_y$. The net effect of the scheme is an evolution

$$v_y^\dagger \exp(-iH_d t)v_y = \exp(-iv_y^\dagger H_d v_y t),$$

i.e., a dynamics according to the Hamiltonian $v_y^\dagger H_d v_y$. We choose a second rotation $u_x$ around the $x$-axis such that $u_x \sigma_a u_x = \sigma_a$ and set $v_x := u_x \otimes u_x \otimes \cdots \otimes u_x$. It is decisive to note that

$$-H_d = v_y^\dagger H_d v_y + v_x^\dagger H_d v_x.$$

This has the interesting consequence that for small times $\epsilon$ one has

$$v_x^\dagger \exp(-iH_d \epsilon)v_y v_y^\dagger \exp(-iH_d \epsilon)v_y \approx \exp(+iH_d \epsilon)$$

up to terms of second order of $\epsilon$. This first order approximation is usually referred to as average Hamiltonian theory \cite{1,3}. The intuitive meaning is that the time evolution according to $H_d$ can be approximatively inverted by dividing the time $t$ into small intervals of length $\epsilon$ and interspersing the natural time evolution by the above pulses. The inverted dynamics is two times slower than the natural one. We express it by saying that the time overhead of inverting the Hamiltonian $H_d$ is 2. The task of time-reversal is a special case of the general problem of simulating Hamiltonians that has recently been considered by several authors \cite{13,14,15}.

Note that the decoupling and inversion schemes for the dipole-dipole Hamiltonian is simple with respect to

*Electronic address: janzing@ira.uka.de
three aspects: (a) it does not use selective pulses, i.e., in each time step the same unitary transformation is applied to all spins. (b) The number of steps of this inversion scheme does not increase with \( n \) since it is always 2, and (3) the time overhead does not increase with \( n \) since it is also 2.

The purpose of this article is to show that there are interactions that are considerably more complex to invert with respect to all three criteria. The most general spin-spin interaction on \( n \) spins is given by

\[
H_J := \sum_{k < l} \sum_{\alpha, \beta} J_{k\alpha, \beta \sigma_a}^{(k)} \sigma_{\beta \sigma_a}^{(l)},
\]

where \( J \) is chosen to be a real symmetric \( 3n \times 3n \)-matrix with zeros for \( k = l \). Note that the symmetry of the coupling matrix \( J \) does not imply any physical symmetry of the interaction. It is a consequence of our redundant notation that turns out to be very useful. The coupling matrix \( J \) consists of \( 3 \times 3 \)-blocks. The \( 3 \times 3 \)-matrix \( J_{kl} \) given by the block at position \((k, l)\) describes the coupling between the spins \( k \) and \( l \). We have \( J_{kl} = J_{lk}^T \), i.e. \( J \) is the transpose of the matrix describing the coupling between the spins \( k \) and \( l \). The blocks on the diagonal are zero matrices.

Let \( \mathcal{C} := SU(2) \otimes SU(2) \otimes \cdots \otimes SU(2) \) be the control group of local operations on the spins. As already mentioned all operations in \( \mathcal{C} \) are assumed to be implemented arbitrarily fast. The most general refocusing scheme (also called time-reversal or inversion) based on the first order approximation above is given by rotations \( v_1, v_2, \ldots, v_N \in \mathcal{C} \), and (relative) times \( t_1, t_2, \ldots, t_N \) such that the average Hamiltonian

\[
\bar{H} := \sum_j t_j v_j^\dagger H_J v_j
\]

is equal to \(-H_J\). Here \( N \) is the number of time steps and \( \tau := \sum_j t_j \) is the time overhead. The time overhead gives the slow-down of the inverted Hamiltonian. In the following we consider both the number of time steps and the time overhead as complexity measures. In contrast, if the sequences are chosen in such a way that the average Hamiltonian is zero one has a decoupling scheme. Each inversion scheme with \( N \) steps defines a decoupling scheme with \( N + 1 \) steps in a straightforward way (note that the notion of time overhead does not make sense for decoupling). Conversely, each decoupling scheme can be converted to an inversion scheme as follows. The equation

\[
\sum_{j=0}^N t_j v_j^\dagger H_J v_j = 0
\]

implies

\[
\sum_{j=1}^N (t_j / t_0) (v_j v_0^\dagger) H_J (v_j v_0^\dagger)^\dagger = -H_J
\]

by elementary calculation. Therefore we shall restrict our attention to inversion.

The condition on inversion schemes can be rewritten by expressing the action of the control operations on the coupling matrix \( J \) as follows. Note that any unitary operation \( u \in SU(2) \) corresponds to a rotation on the 3-dimensional Bloch sphere via the relation

\[
u^\dagger \left( \sum_{\alpha} c_\alpha \sigma_\alpha \right) u = \sum_{\alpha} \tilde{c}_\alpha \sigma_\alpha,
\]

where the vector \( \tilde{c} = (\tilde{c}_x, \tilde{c}_y, \tilde{c}_z) \) is obtained by applying a rotation \( U \in SO(3) \) on the vector \( c = (c_x, c_y, c_z) \). It is straightforward to verify that conjugation of \( H_J \) by \( v := u^{(1)} \otimes u^{(2)} \otimes \cdots \otimes u^{(n)} \) corresponds to conjugation of \( J \) by a block diagonal matrix of the form

\[
V := U^{(1)} \otimes U^{(2)} \otimes \cdots \otimes U^{(n)} \in \bigoplus_{k=1}^n SO(3).
\]

The condition for time inversion is hence given by

\[
-J = \sum_j t_j V_j J V_j^T,
\]

where the orthogonal matrix \( V_j \) corresponds to the unitary transformation \( v_j \) for \( j = 1, \ldots, N \). Time reversal and decoupling schemes that apply for general coupling \( J \) have been presented in [10,9]. These schemes can even be used when the coupling \( J \) is unknown. Here we focus on optimality criteria for schemes referring to specific couplings and show that there are interactions that cannot be inverted significantly more efficiently than an unknown interaction.

We restrict our attention to interactions with an additional symmetry, namely a Hamiltonian of the following form

\[
H := \sum_{k < l} w_{kl} \sum_{\alpha, \beta} A_{\alpha \beta}^{(k)} \sigma_{\alpha \sigma_a}^{(l)}.
\]

The matrix \( W := (w_{kl}) \) is a real symmetric \( n \times n \)-matrix with zeros on the diagonal. It describes the coupling strengths and the signs of the interactions between all spins. The matrix \( A := (A_{\alpha \beta}) \) is a real symmetric \( 3 \times 3 \)-matrix characterizing the type of the coupling. This means that all spins interact with each other via the same interaction and that only the coupling strength and the sign varies. It is important that in this special case the coupling matrix \( J \) can be expressed as a tensor product of \( W \) and \( A \), i.e. \( J = W \otimes A \).

The matrix \( W \) characterizes the coupling topology of the spins. In the language of graph theory the matrix \( W \) is the adjacency matrix of a weighted graph. Therefore many results on graph spectra (eigenvalues of the adjacency matrices) can be used to derive lower and upper bounds on the number of time steps and the time overhead.

To discuss the complexity aspects we distinguish between the following three cases:
1. $A$ is traceless.

All spins can be subjected to the same transformations in each time step, the number of time steps and the time overhead are at most 2.

2. $A$ has negative and positive eigenvalues but $\text{tr}(A) \neq 0$.

The spins have to be addressed separately, the number of time steps necessarily grows for increasing $n$. But the time overhead does not depend on $n$. It depends only on the eigenvalues of $A$.

3. $A$ is either positive or negative semidefinite, i.e., the non-zero eigenvalues have the same sign.

Then the spins have to be addressed separately, the number of time steps is at least $n-1$, and the time overhead is also at least $n-1$.

To prove these statements we assume w.l.o.g. that the interaction between all pairs is of the form

$$a_x \sigma_x \otimes \sigma_x + a_y \sigma_y \otimes \sigma_y + a_z \sigma_z \otimes \sigma_z,$$

where $a_x, a_y, a_z$ are the eigenvalues of $A$. This can always be achieved by rotating the reference frame.

**Case 1.** Assume $A$ to be traceless. Let $S$ be a rotation in the Bloch sphere that realizes the cyclic permutation of the axis according to $x \to y \to z \to x$. Then we have

$$\sum_{j=0}^{2} V_j J V_j^T = 0,$$

where $V := S \oplus S \oplus \cdots \oplus S$ and $V_j$ is the $j$th power of $V$. Here $S$ is a rotation in the Bloch sphere that realizes the cyclic permutation of the axis according to $x \to y \to z \to x$. The $j$th power of $V$ is denoted by $V^j$. Hence the Hamiltonian is inverted by a sequence of length 2. Due to the equation

$$-J = V J V^T + V^2 J V^2 T$$

the time overhead of this inversion scheme is 2.

**Case 2.** The fact that the spins have to be addressed separately has also been noted in [13]. It can be seen as follows. If all spins are subjected to the same transformation each $3 \times 3$-block of $J$ is conjugated by an element of $SO(3)$. Such a conjugation preserves the trace of each block matrix. This trace is even preserved under positive linear combination, i.e. the trace of each resulting $3 \times 3$ matrix has the same sign as the trace of the original matrix. Therefore a sequence applying the same transformation to all spins can never change the sign of the trace in any block. But this is required for obtaining the inverse entries.

We show that the number of time steps cannot be constant, i.e. independent of $n$. Assume w.l.o.g. that $tr(A) > 0$. Choose a partition of $SO(3) = S_1 \cup S_2 \cup \cdots \cup S_p$ into equivalence classes such that for any pair $O_i, O_j \in S_i$ $(i = 1, \ldots, p)$ implies $tr(O_i O_j^T) \geq 0$ ($p$ depends on $A$). This is always possible since the partition can be chosen in such a way that all orthogonal transformations in the same class are sufficiently close together. Then $O_i O_j^T$ almost corresponds to a conjugation of $A$ by an orthogonal matrix and its trace cannot deviate too much from $tr(A)$ due to the continuity of the trace.

Let $O_j(k) \in SO(3)$ be the operation performed on the $k$th spin in time step $j$ (described as action on the coupling matrix). In each time step at least $\lceil n/p \rceil$ spins are transformed by operations of the same class. After $N$ time steps at least $\lceil n/p \rceil^N$ spins have been transformed by operations of the same class in each step. Let $k$ and $l$ be such a pair that has been transformed by operations of the same equivalence class in each time step. Then the trace of the average coupling between the spins $k$ and $l$ after the sequence is given by

$$tr(\sum_j t_j O_j(k) A O_j(l)^T) \geq 0.$$  \hspace{1cm} (2)

If the sequence is an inversion scheme then we must have

$$\sum_j t_j O_j(k) A O_j(l)^T = -A.$$

But this condition contradicts the inequality (3)\textsuperscript{1}. Therefore such a pair $k$ and $l$ must not exist. This gives the lower bound $N \geq \log n/\log p$ on the number of time steps $N$.

We show that the time overhead does not depend on $n$. We assume w.l.o.g. $a_x > 0 > a_z$ for the eigenvalues of $A$. First we describe a partial decoupling scheme selecting for instance the $\sigma_z \otimes \sigma_z$ coupling terms while switching off the $xx$ and $yy$ terms. Following [3] such a decoupling can be achieved by certain sequences of local conjugations by the unitary $i\sigma_z$. Each time step of this scheme is described by a column of a Hadamard matrix. The entries determine which spins are conjugated by $i\sigma_z$ transformations. The idea is that the $xx$ and $yy$ terms acquire in exactly half of the time steps a minus sign. Note that this scheme does not weaken the $zz$ coupling. In other words, although this scheme requires a number of *time steps* of the order $n$ the *time overhead* for the simulation of the interaction $\sum w_{kl} a_z \sigma_z^{(k)} \sigma_z^{(l)}$ by the original one is 1.

\hspace{1cm}

\textsuperscript{1}Here $\lceil x \rceil$ denotes the smallest integer $m$ such that $x \leq m$. 

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Hence, we conclude that the rank of the right hand side is at least $\lambda_{\min}$, where $\lambda_{\min}$ is the minimal eigenvalue of $W$. Therefore the rank of $W$ is at least the number of positive eigenvalues of $-W \otimes A$. Since $\lambda_{\min}$ is not negative we can reverse similarity $W$ with time overhead $-a_y/a_z$.

To invert the $zz$-components we use the $xx$-components. The time overhead is $-a_z/a_x$. In summary we see that the time overhead is independent of $n$. It only depends on the eigenvalues of $A$.

**Case 3.** Let $t_1, t_2, \ldots, t_N$ be the (relative) times and $V_1, V_2, \ldots, V_N$ with $V_j \in \bigoplus_{k=1}^n SO(3)$ be the operations of an inversion scheme, i.e.,

$$\sum_j t_j V_j (W \otimes A) V_j^T = -W \otimes A. \quad (3)$$

First note that an inversion scheme for a given Hamiltonian $H_t$ can also be applied to a rescaled Hamiltonian obtained by changing the strength and the sign of an arbitrary spin pair interaction. If all the coefficients $w_{kl}$ are non-vanishing for $k \neq l$ then we can equivalently describe a time inversions scheme for the coupling matrix $J := W \otimes A$ where all non-diagonal entries of $W$ are 1 and the diagonal consist of zeros. Hence the fact that interactions decrease with distance of the spins is irrelevant for considerations of the complexity of time inversion (as long as the interaction cannot be neglected). Therefore we assume w.l.o.g. all non-diagonal entries of $W$ to be 1.

For each time step let $V_j$ be the block diagonal matrix $V_j = U_j^{(1)} \oplus \cdots \oplus U_j^{(n)}$. Set $R := \sum_{j=1}^N t_j V_j (1 \otimes A) V_j^T$. We add $R$ to both sides of eq. (3) and obtain

$$\sum_{j=1}^N t_j V_j ((W + 1) \otimes A) V_j^T = -W \otimes A + R. \quad (4)$$

The rank of the matrix $(W + 1)$ is 1 since all its entries are 1. Consequently, the rank of the left hand side of equation (4) is at most $N r$, where $r$ is the rank of $A$. Note that $R$ is a semi-positive matrix. Therefore the rank of the right hand side is at least the number of positive eigenvalues of $-W \otimes A$. The matrix $-W$ has $n-1$ positive eigenvalues (by adding the identity to $W$ one easily verifies that $W$ has the eigenvalues $n-1, -1, 1, \ldots, -1$). Hence $-W \otimes A$ has $(n-1)r$ positive eigenvalues. We conclude that the rank of the right hand side is at least $(n-1)r$. This proves the statement $N \geq n - 1$.

We show now that the time overhead also grows with $n$. Let $\lambda_{\min}$ and $\lambda_{\max}$ be the minimal and maximal eigenvalues of $J$, respectively. Note that $\lambda_{\min}$ is negative since $J$ is traceless. Let $t_1, t_2, \ldots, t_N$ be the (relative) lengths of the time steps. Then we have

$$\sum_j t_j \lambda_{\max} \leq -\lambda_{\min},$$

since the maximal eigenvalue of the sum of matrices in eq. (4) is at most the sum of their maximal eigenvalues and $-\lambda_{\min}$ is the maximal eigenvalue of $-J$. We conclude that the time overhead $\tau := \sum_j t_j$ for the inverse evolution is at least

$$\tau \geq -\lambda_{\max}/\lambda_{\min}.$$

Since the maximal and minimal eigenvalues of $W$ are $(n-1)$ and $-1$, respectively, the maximal and minimal eigenvalues of $J$ are $(n-1)a_{\max}$ and $-a_{\max}$ where $a_{\max}$ is the maximal eigenvalue of $A$. We conclude that the minimal time overhead is at least $n - 1 \square$.

The truncated dipole-dipole coupling is an example for case 1. The corresponding matrix $A$ is given by

$$A := \text{diag} (1, 1, -2).$$

An important example for case 3 is the strong scalar coupling where $A$ is the identity matrix. By combining both types one can easily find examples for case 2 $\square$.

Besides the practical applications of refocusing the lower bounds on the inversion complexity may be seen as a small contribution to the old debate on the origin of phenomenological irreversibility: Whereas the considered dynamical evolutions are strictly reversible the complexity of a real implementation of the time inversion is growing with the number of interacting particles. Note that the relevance of complexity theory for the definition of physical entropy has been advocated for by several authors $\square$. Of course our complexity bounds are restricted to the assumptions of average Hamiltonian theory. Inversion schemes that are not based on this approach and include higher order terms of the Magnus expansion may be less complex. However, our results present an example how to develop a complexity theory of time reversal in physics.

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