Robust Entanglement in Anti-ferromagnetic Heisenberg Chains by Single-spin Optimal Control

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(Dated: March 16, 2010)

We demonstrate how near-perfect entanglement (in fact arbitrarily close to maximal entanglement) can be generated between the end spins of an anti-ferromagnetic isotropic Heisenberg chain of length $N$, starting from the ground state in the $N/2$ excitation subspace, by applying a magnetic field along a given direction, acting on a single spin only. Temporally optimal magnetic fields to generate a singlet pair between the two end spins of the chain are calculated for chains up to length 20 using optimal control theory. The optimal fields are shown to remain effective in various non-ideal situations including thermal fluctuations, magnetic field leakage, random system couplings and decoherence. Furthermore, the quality of the entanglement generated can be substantially improved by taking these imperfections into account in the optimization. In particular, the optimal pulse of a given thermal initial state is also optimal for any other initial thermal state with lower temperature.

PACS numbers: 03.67.Hk,03.67.Lx,7510.Pq,78.67.Lt

I. INTRODUCTION

Spin systems are important models to understand many-body physics and to investigate many interesting problems in the area of quantum information processing [1]. Coherent control of such systems to achieve certain key tasks such as entanglement generation is one of the main problems in quantum mechanics. There have been several proposals already for entanglement generation between the end points of a spin chain both by distributing the entanglement through the chain [2,3] and entanglement generation through a quench followed by the natural non-equilibrium dynamics of the system [4–6]. Unfortunately, the attainable entanglement in these schemes is not maximal and achieving an arbitrarily high entanglement between ending spins demands more control. Although there has been significant progress in both the theory and implementation of coherent control, the microscopic nature of most quantum objects makes it difficult to control all elements of the system individually. Local addressing of individual spins, for example, remains a significant challenge. Applying fields that globally address the entire system is one way to avoid such problems [7]. On the other hand, if assuming locally addressing ability of a many-body system, one interesting question is what is the minimal controlling resource that can perform certain desired task. For example, universal quantum computation can be achieved through controlling a small part or gateway of the whole system [8–12], when the system intrinsic Hamiltonian provides the necessary non-local interactions for a successful control. Aside from not requiring access to the entire system, limiting the interaction of the controller with the system can be advantageous as quantum coherence is very fragile and any incoherent interaction with a macroscopic control apparatus can contribute to decoherence. Minimal control is therefore likely to reduce controller-induced decoherence, which is a limiting factor for many quantum information tasks. It has been shown that a wide class of coupled many-body systems can be manipulated as required by controlling a local subsystem [8], and even for generic (not necessarily multi-partite) systems, control of a small subspace or even single transition is often sufficient to achieve full controllability [13]. In particular, the XXZ-Heisenberg model is controllable if one end spin can be fully controlled [9].

Controllability, however, only guarantees the existence of a control to complete a certain task, but does not tell us how to generate such a control, and even constructive controllability proofs do not usually result in efficient solutions. Efficiency is critical due to limited coherence time for many systems, which makes long pulse sequences problematic. Moreover, practical feasibility considerations impose various constraints on the permissible fields, from rise time to the complexity of its frequency spectrum. Consequently, control design has to be considered case by case and there is no general scheme that is optimal for an arbitrary system. Recently, there have been several proposals for achieving certain tasks in quantum information. For instance, an efficient transfer of quantum states can be achieved in an Ising chain, which is accessible in Nuclear Magnetic Resonance (NMR), through global [7] and mixture of global-local [14] pulses. In [15], a realistic scheme is proposed to achieve high fidelity state transfer by applying a sequence of two-qubit gates at one end of the chain and it was shown that the two qubit gates can be implemented by a proper sequence of switching the interaction of the two spins. Universal quantum computation along the XY spin chain can be achieved by controlling the two spins at one end of the chain [10,12]. In [10] one spin is controlled by two independent magnetic fields and a fast Hadamard gate operating on the other spin. Alternatively, in [12] the two spins are controlled via three independent control fields, two of which are non-local interactions. Also, very recently, almost perfect state transfer has been achieved by controlling the magnetic field in the $z$ direction over all spins in the ferromagnetic...
Heisenberg chain [16].

In this work, we consider the problem of entanglement generation between the two ends of an anti-ferromagnetic Heisenberg spin chain when control is restricted to a uni-directional local magnetic field on one spin at either end of the chain. This type of control is not sufficient for full controllability of the \( N \)-spin system [15] as both the system and control Hamiltonian are excitation preserving, and thus the system decomposes in into \( N + 1 \) excitation subspaces. For a Heisenberg chain, we shall demonstrate that with the Heisenberg interaction and the local control Hamiltonian, the system is controllable in the particular subspace with the largest number of excitations, and thus if the target state is in the same subspace as the initial state, it is reachable by such local control. Through optimization, we find the time-varying control field that generates an almost perfect singlet pair between two ends of the chain, after the system is initially prepared in the ground state. In general, calculations to generate the optimal control field for the largest excitation subspace of the anti-ferromagnetic chain are considerably more demanding than the more common single-excitation subspace calculations [16], as the system state lies in the \( N/2 \)-excitation subspace for \( N \) even, which has dimension \( N!/(N/2)!^2 \) as opposed to dimension \( N \) for the first excitation subspace, and has a complicated form being a superposition of many computational basis states. Considering this scenario, however, has several benefits from a practical perspective: (i) most realizations of spin chains are anti-ferromagnetic in their nature [17]; (ii) in our entanglement generation strategy the initial state is the ground state of the system, which any system naturally takes when it cools down and thus there is no need for extra control to initialize the system; (iii) since the ground state of the system is highly entangled it can be considered as an initial source for quantum information tasks. This helps simplify the control mechanism as multipartite entanglement naturally exists and the control simply has to convert it to utilizable bipartite entanglement between the distant end spins. Despite the highly restrictive nature of the control and the dimension of the state space, we find that the resulting controls are robust with regard to several non-ideal features such as thermal fluctuations, decoherence, leakage of the local magnetic field and existence of uncertainty in the couplings of the system.

The paper is organized as follows: in Section II, we briefly introduce the model and its invariant excitation subspace characterized by a definite value of the total excitations. In Section III, we will formulate the entanglement generation task into an optimization problem, and numerically find the optimal control pulses. In Section IV, from controllability point of view we provides some analysis trying to understand why such proposed optimization process can generate the required control. In Section V, we add some more practical conditions to the problem and discuss how these extra conditions will affect the control results. The results are summarized in the section VI.

II. SYSTEM AND CONTROL MODEL

We consider an isotropic Heisenberg chain of \( N \) spin-\( \frac{1}{2} \) particles with the nearest-neighbor interaction:

\[
H_s = J H_0 = J \sum_{n=1}^{N-1} (X_n X_{n+1} + Y_n Y_{n+1} + Z_n Z_{n+1}),
\]

(1)

where the Pauli operators are defined as usual

\[
X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.
\]

\( J \) is the coupling between adjacent spins, and is positive for an antiferromagnetic chain. Let \(|0\rangle\) and \(|1\rangle\) be the basis vectors of a single spin, representing the spin-down and spin-up states. The \( 2^N \)-dimensional Hilbert space \( \mathcal{H} \) of the spin chain is spanned by tensor products of the \( N \) single spin basis vectors, the computational basis states, for which we shall use the shorthand notation \(|0\ldots0\rangle = |0\rangle^\otimes N \), etc. For each basis state the number of excitations is simply the number of \(|1\rangle\)'s in that basis. For instance \(|11\ldots1\rangle\) has \( N \) excitations. Setting \( S_2 = \sum_{n=1}^{N} Z_n \), it is easy to verify that \(|H_0, S_2\rangle = 0\), hence \( H_0 \) is invariant on every excitation subspace. Accordingly, \( \mathcal{H} \) can be written as a direct sum of \( N + 1 \) excitation subspaces \( \mathcal{H}_n \) \((n = 0, \ldots, N)\) whose basis vectors are those having \( n \) excitations. The dimension of \( \mathcal{H}_n \) is \( \binom{N}{n} \). For chains with an even number of spins the system \(|1\rangle\) has a unique ground state in the \( \frac{N}{2} \)-excitation subspace \( \mathcal{H}_{N/2} \). For odd-length chains the ground state is doubly degenerate with one ground state in the \( \mathcal{H}_{(N−1)/2} \) and \( \mathcal{H}_{(N+1)/2} \) subspace each.

Next, we impose a local magnetic field along the \( z \)-direction on the left end spin, with the resulting Hamiltonian:

\[
H_c = B(t) H_1 = B(t) Z_1
\]

(2)

where \( B(t) \) is the magnitude of \( H_c \), which can be varied over time. For spin chains comprised of coupled quantum dots, such an interaction could be achieved using local voltage gates. This is the Hamiltonian we shall control for entanglement generation. The direction of field is not essential due to the symmetry of the Heisenberg Hamiltonian. The main idea is to demonstrate that perfect end-to-end entanglement can be generated from only a local magnetic field along a given direction. This requirement is experimentally simpler than other proposals where independent control fields along different directions are required. Of course, the more controllable degrees of freedom, the more type control tasks can be completed, but a single unidirectional local field is sufficient for entanglement generation, and indeed controllability on the \( N/2 \)-excitation subspace as we shall see.

The total Hamiltonian of the spin chain thus becomes

\[
H(t) = H_s + H_c = J H_0 + B(t) H_1.
\]

(3)

Since \( H_1 \) is invariant on every excitation subspace \( \mathcal{H}_M \), \( H(t) \) is also invariant on these subspaces. As a result the number of excitations of a given initial state \(|\psi(t)\rangle\) does not change under the evolution

\[
\frac{d}{dt} |\psi(t)\rangle = -i H(t) |\psi(t)\rangle,
\]

(4)
i.e., if $|\psi(0)\rangle$ is in the $M$-excitation subspace then $|\psi(t)\rangle$ will be in $\mathcal{H}_M$ for all $t$. Throughout this paper we choose units such that $\hbar = 1$, so $J$ and $B(t)$ has the dimension of frequency. For NMR experiments $J$ is typically a few hundred Hz, and $B(t)$ is around 50 kHz for liquid-state NMR and a few hundred kHz for solid-state NMR [18].

III. OPTIMAL CONTROL DESIGN

Our question is whether we can find an appropriate control pulse $B(t)$ in the model (3) to generate a maximally entangled state between the two end spins at a certain final time $t = t_f$. We shall first assume that the system is initialized in the ground state $|G_0\rangle$ of $H_0$ and thus in a pure state. In principle, this can be done by simply cooling the systems and this assumption will later be relaxed. As mentioned above, for even chains the ground state of $H_0$ is unique and lies in the subspace of $\mathcal{H}_{N/2}$ so that cooling the system is enough to prepare it. For chains of odd length the degeneracy can be lifted by applying a small global magnetic field during the cooling process and the system can be prepared into the ground state in the subspace $\mathcal{H}_{(N+1)/2}$. In the following, for simplicity, we will call $\mathcal{H}_{N/2}$ for even chain and $\mathcal{H}_{(N+1)/2}$ for odd chain as the largest excitation subspace, and we assume the system is initially prepared as the ground state $|G_0\rangle$ in the largest excitation subspace.

The control objective is to find a time-varying control field $B(t)$, $t \in [0, t_f]$, such that the final state at time $t_f$ takes the form

$$|\psi(t_f)\rangle = |\psi^\rangle_{1,N} \otimes |\psi^\rangle_{re},$$

where $|\psi^\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$ is the singlet state between the first and the last spin, and $|\psi^\rangle_{re}$ is the state of the remainder, i.e., spins $n = 2, 3, ..., N-1$, on which we do not impose any constraint.

One of the methods to generate the control pulse $B(t)$ is through optimization, where the target state $|\psi(t_f)\rangle$ is the maximal (or minimal) point of a certain objective function $K[B(t)]$. A good candidate in our case is

$$K[B(t)] = \langle \psi(t_f) | A | \psi(t_f) \rangle,$$

where the operator $A$ is the projection onto the target subspace

$$A = |\psi^\rangle_{1,N} \langle \psi^| \otimes I_{re},$$

and $|\psi^\rangle_{1,N} \langle \psi^|$ is the density operator for the singlet state between spins 1 and $N$, which we desired to prepare, and $I_{re}$ is the identity operator acting on the rest part of the chain. Eq. (6) shows that this function is the fidelity of the density matrix of the end spins $\rho_{1,N}(t)$ with respect to the singlet state at time $t_f$. Consequently, this function is always positive and assumes its maximum for states of the form (5), where the two end spins form a singlet. Hence, our main goal is to drive this system to its maximum by varying $B(t)$ over the time interval $[0, t_f]$. For simplicity, we will vary $B(t)$ in the function space of the piecewise-constant functions.

The optimization procedure is as follows. We divide the time $[0, t_f]$ into $p$ equally spaced sub-intervals, $\Delta t = t_f/p$. On each time interval the control field $B(t)$ takes the constant value $B_m$ ($m = 1, 2, ..., p$) satisfying $|B_m| < B_M$, where $B_M$ is the maximum amplitude of the control field that we can generate experimentally. Assuming unitary evolution governed by the Schrödinger equation, the final state subject to this piece-wise constant control is simply

$$|\psi(t_f)\rangle = U(B_p) \cdots U(B_1)|G_0\rangle,$$

where

$$U(B_m) = e^{-iu(JH_0 + B_m H_1)\Delta t},$$

and the fidelity is simply a function of $p$ variables, $K[B(t)] = K[B_1, \ldots, B_p]$. This is a standard optimization problem in a finite-dimensional parameter space, which can be solved using various methods. We use a quasi-Newton method developed by Boyden, Fletcher, Goldfarb and Shanno [20] (BFGS), which is an improvement over the standard GRAPE algorithm [19] widely used for quantum control problems.

The algorithm is summarized as follows: (1) Choose an initial trial function $B(t) = B^{(1)}(t)$, which could be constant $B^{(1)}(t) = 1$ or some other random choice. (2) Iteratively generate $B^{(m+1)}(t)$ from $B^{(m)}(t)$ by applying the quasi-Newton method, which guarantees $K[B^{(m+1)}(t)] > K[B^{(m)}(t)]$. The algorithm is terminated if the change of the fidelity is smaller than a given threshold, or we cannot find a search direction to increase the fidelity further. The method guarantees that the function sequence $B^{(m)}(t)$ converges to a local maximum $B_{max}(t)$ of the function $K[B(t)]$, and constraints, e.g., on the field amplitudes, can be explicitly taken into account. In applications such as NMR where the field amplitudes $B(t)$ can be large compared to $J$ (at least $10^2 - 10^3$ J) it is usually not necessary to impose explicit amplitude constraints — at least our simulation results for this problem suggest that the amplitudes of the optimized fields are usually well below 100 J if we start with an initial field $B^{(1)}(t)$ close to the zero field $B = 0$, as is to be expected for a local optimization method. Therefore in most of the following calculations no amplitude constraints have been imposed, except where otherwise stated. In general amplitude constraints increase the amount of time required to reach the objective but the imposition of such constraints can be beneficial by increasing the robustness of the optimal pulses obtained with regard to noise, field leakage, etc. Beside the fidelity $K[B(t)]$ of the final state with respect to the desired singlet state, we also use the entanglement measured by the concurrence [21] to quantify the quality of our procedure, where the entanglement $C$ is maximal ($C = 1$) if we successfully generate a perfect singlet.

Using this optimal control framework we computed optimal pulses for spin chains of length $N = 4$ to 20. An example of an optimal control field and the corresponding evolution of the system for $N = 4$ is shown in Fig. I. The control steers the ground state of $H_0$, which is a superposition of all six computational basis states in the $N/2 = 2$ excitation subspace $\mathcal{H}_2$, to a $+1$-eigenstate of the observable $A$ in the same subspace. For $N = 4$ the $+1$-eigenspace of $A$ restricted to $\mathcal{H}_2$.
is spanned by \( \{ \frac{1}{\sqrt{2}} (|0011\rangle - |1010\rangle), \frac{1}{\sqrt{2}} (|0101\rangle - |1100\rangle) \} \) and the control must steer the initial state to some state in this subspace. In the example shown in Fig. 1 for instance, virtually all the population is transferred to the eigenstate \( |\psi\rangle = \frac{1}{4} (|0011\rangle - |1010\rangle - |0101\rangle + |1100\rangle) \) at the final time, although the population of the target state and the concurrence between the end spins do not increase monotonically unlike for some local optimization approaches \[22\]. The partial trace of the final state over the inner spins (up to three digits accuracy) is

\[
\rho_{14} = \text{Tr}_{2,3}(|\psi\rangle\langle\psi|) = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & -0.501 & -0.500 \\
0 & -0.500 & 0.499 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix},
\]

which is an almost perfect Bell state with concurrence 0.99998, and we can achieve fidelities and concurrences almost arbitrarily close to 1 by relaxing the constraints on the field amplitudes, pulse duration or time resolution of the fields slightly. In this sense we claim that this method can generate perfect entanglement.

Although the dimension of the \( \frac{N^2}{4} \) -excitation subspace increases from \( \binom{4}{2} = 6 \) for \( N = 4 \) to \( \binom{20}{10} = 184,756 \) for \( N = 20 \), rendering the optimization problem considerably more challenging and time-consuming, we are still able to find optimal optimal pulses for which \( K[B] \) assumes values very close to 1 in relatively short time, suggesting that our optimization method for generating end-to-end entanglement is still effective for relatively long spin chains. For a given chain there is always a lower bound \( T_C \) for the evolution time \( t_f \), however, below which we can never achieve unit fidelity no matter how many time steps or iterations are used. Unfortunately, analytical expressions for these bounds are known only for very simple systems. We therefore numerically explore the search space to find approximate lower bounds \( T_C \) as a function of the chain length \( N \). The results, shown in Fig. 2 suggest a quadratic increase with respect to chain length \( N \), similar to what was reported in \[10\] for implementing the universal quantum computation by controlling two qubits of an XY chain, rather than a linear increase as in some other entanglement generating schemes \[3, 4\] where entanglement propagates from one end through the chain. The nonlinear dependence on the length of the chain is not surprising as the mechanism for increasing the entanglement between the end spins in our scheme involves dynamic population transfer from the ground state of \( H_0 \) to an eigenstate of the observable \( A \). We note that the control itself cannot create entanglement directly as the control Hamiltonian \( H_1 \) is completely local. It can only alter the entanglement between the end spins by taking advantage of the existing interactions between all spins and the resulting non-trivial dynamics.

\[\text{FIG. 1:} \text{Color online} \text{ (a) Example of optimal field } B_6(t) \text{ for } N = 4 \text{ and (b) corresponding evolution of the populations of the computational basis states in the 2-excitation subspace and the population } p(t) \text{ of the state } |\psi\rangle \text{ (thick solid line) and (c) concurrence } C_{14}(t) \text{ between spins 1 and 4. The evolution shows that the pulse transfers virtually all population to the state } |\psi\rangle, \text{ which exhibits perfect entanglement between the end spins, as demonstrated by the concurrence of the reduced density matrix. (Pulse shown obtained with amplitude constraint } |B(t)| / J \leq 1. )\]

\[\text{FIG. 2:} \text{Color online} \text{ Lower bound on the time } T_C \text{ required for generating entanglement in terms of } N^2, \text{ based on numerical optimization results for chains of lengths } N = 4 \text{ to } 15 \text{ without constraints.}\]

\[\text{IV. CONTROLLABILITY & REACHABILITY CONSIDERATIONS}\]

Considering the restrictions imposed on the control, it is rather surprising that we are able to find optimal control solutions at all, and it is worthwhile to investigate whether there always exist controls that achieve perfect entanglement, at least in principle. In order to answer these questions, we need to review the concepts of reachability and controllability. Ultimately, the question we would like to answer is what is the set of states that is reachable from the ground state for a system governed by the evolution \[4\]. We already know that there are some constraints. For a Hamiltonian system the spectrum...
of the density operator is invariant. For pure initial states this simply means that the set of reachable states is a subset of the pure states. We also know that there are additional limitations as both $H_0$ and $H_1$ in our case commute with total excitation operator $S_z$, and hence the Hilbert space decomposes into excitation subspaces on which the dynamics is invariant. Thus if the initial state is a pure state on the $N/2$ excitation subspaces then the set of reachable states is a subset of the pure states on this excitation subspace. However, the key question is whether the target state $|\psi\rangle$ in this excitation subspace is reachable from the initial state $|G_0\rangle$. Unfortunately, this is a very difficult question to answer directly in general, except for controllable systems. We must be careful here as there are different degrees of controllability [23] but if we can show, for instance, that the unitary evolution of the system is controllable, then pure-state controllability follows.

The Schrödinger equation (4) can be rewritten into an equation in terms of the unitary process $U(t)$ as the variable

$$\dot{U}(t) = -i(JH_0 + B(t)H_1)U(t)$$

where $U(0) = I$ and the solution for a given control $B(t)$ is denoted as $U(t, B(t))$. In this context, the reachable set $R$ is defined as the set of unitary matrices that can be achieved by the dynamics $U(t, B)$ for some (admissible) control $B(t)$, i.e., $U \in R$ if and only if there exists an admissible control $B(t)$ such that $U(t_f, B(t)) = \hat{U}$ and we have the following [24]:

**Theorem 1.** Let $L$ be the Lie algebra generated by $span\{-iH_0, -iH_1\}$, often called the dynamical Lie algebra. Then $R = e^L$.

Thus, the reachable set depends on the dynamical Lie algebra generated by the Hamiltonian. If $L = U(2^N)$ or $L = SU(2^N)$, then $R = U(2^N)$ or $R = SU(2^N)$ and the system is controllable in the sense that we can implement any unitary process up to a global phase and steer any density operator to any other density operator with the same spectrum. Back to our spin chain problem, for $H = JH_0 + B(t)H_1$ with $H_0$ and $H_1$ as in Eqs (1) and (2), if the system is controllable on $H_{N/2}$ for even or $H_{(N+1)/2}$ for odd $N$, then the existence of the control to generate the required singlet state is guaranteed. A straightforward way to check controllability is by calculating the dimension of the dynamical Lie algebra. Calculations for small chains of different length suggest full controllability on the relevant excitation subspaces for chains of both even and odd length. However, such calculations are laborious and impractical for long chains. Similarly, proving that the dimension of the dynamical Lie algebra is $M^2$, where $M$ is the dimension of the $H_{N/2}$ or $H_{(N-1)/2}$ excitation subspace, for any $N$ is a difficult mathematical problem. However, for even-length isotropic Heisenberg chains, controllability can be easily verified using the following useful result [25]:

**Theorem 2.** If $H_0$ is effectively strongly regular and $H_1$ is connected, then the system is controllable.

Here $H_0$ is strongly regular if all the transition frequencies $\omega_{kl} = e_k - e_l$, where $e_k$ are the eigenvalues of $H_0$, are distinct. Choosing a basis such that $H_0$ is diagonal, $H_0 = diag(e_1, e_2, \ldots, e_n)$, let $H_1 = (b_{ij})$ be the matrix representation with respect to this basis. $H_1$ is connected if the graph represented by $H_1$ is a connected graph. To be more specific, we say the indices $j$ and $k$ are connected if $b_{jk} \neq 0$, and if every two indices are connected through several nonzero $b_{jk}$’s, then $H_1$ is called connected. Moreover, $H_0$ is called effectively strongly regular if $\omega_{jk}, j \neq k$, are nonzero and distinct whenever $b_{jk} \neq 0$. Using these definitions and the previous theorem we can verify on a case by case basis that even-length Heisenberg chains are controllable on $H_{N/2}$.

**Example 1.** For $N = 4$ we have $dim(H_2) = 6$, $H_0$ and $H_1$ take the following forms in the eigenbasis of $H_0$:

$$H_0 = \begin{pmatrix} -2\sqrt{3} -3 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2\sqrt{2} -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\sqrt{3} -3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2\sqrt{2} -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix},$$

$$H_1 = \begin{pmatrix} 0.81 & 0 & 0 & 0.50 & 0 & -0.31 \\ 0.58 & 0 & 0 & -0.58 & 0 & 0.58 \\ 0.50 & -0.58 & 0 & -0.65 & 0 & 0.75 \\ 0 & 0.31 & 0.58 & 0 & -0.75 & 0 \end{pmatrix},$$

which shows that $H_0$ is effectively strongly regular and $H_1$ is connected. Therefore, the system is controllable on the $H_2$ excitation subspace, and by virtue of controllability any pure state in the $H_2$ excitation subspace is reachable from the ground state $|G_0\rangle$, including our target Bell state $|\psi\rangle$.

We can similarly verify that the systems governed by (3) satisfy the criteria for controllability above on $H_{N/2}$ for $N$ even ranging from 4 to 16. For longer chains, such verification will become inefficient again due to the evaluations of eigenvalues and eigenvectors for large matrices. For odd $N$, $H_0$ ceases to be effectively strongly regular on the $(N + 1)/2$ excitation subspace for $N > 3$, and the above theorem does not apply. However, this does not imply non-controllability as the above controllability criteria is only sufficient but not necessary. In fact direct calculation of the dimension of the dynamical Lie algebra for odd chains suggests that the system is still controllable. For instance, for $N = 5$ we obtain $dim(H_2) = (\binom{5}{2} = 10$ and direct computation of the Lie algebra shows that it has dimension $100 = 10^2$, suggesting that the Lie algebra in this case is $\text{u}(10)$, which implies full controllability on the subspace.

Although controllability implies reachability and the existence of a control that steers the initial state to the target state, it should be noted that it does not answer the question of the minimal time required to steer the system to the target state. Furthermore, in practice the finite time resolution of the field and bounds on the field strengths impose additional constraints, i.e., even if there exists an unbounded control that steers the initial state to the target state in time $t_f$, ...
there may not be a piecewise constant solution of the form \((B_m) = (B_1, \ldots, B_p)\) if \(p\) is fixed and \(|B_m| \leq B_M\) for some fixed bound \(B_M\). Finally, most optimization techniques including the quasi-Newton-method used in the previous section are only guaranteed to find some extremum of the objective function, which need not necessarily correspond to a global optimum.

For more general spin chain models, for example, the XXZ chain, we can still use the above optimization method to generate perfect entanglement. For different length of chains we have calculated, the system is always found to be controllable on the subspace in question. More interestingly, for XX chain, such optimization method can also generate perfect entanglement from the ground state, but the system is found to be non-controllable on that subspace. This gives an example where the perfect end-to-end entangled state is reachable from the ground state, but controllability does not hold, a strong evidence that reachability is weaker than controllability.

V. CONTROL PERFORMANCE UNDER REALISTIC CONDITIONS

In the previous sections we have illustrated that a single magnetic field in the \(z\)-direction acting on a single spin suffices to generate a perfect entanglement between two ends of a Heisenberg chain. However, the optimal control design is based on four ideal assumptions, namely that

1. The system can be prepared in its ground state;
2. The control field can locally address a single spin without affecting the others;
3. The system is homogeneous, i.e., all couplings are equal and the coupling strength is known;
4. The system is isolated from its environment.

In this section we consider how the effectiveness of the optimal controls is affected when these assumptions are relaxed.

A. Thermal Initial State

In an ideal setup we would be able to cool the system to its ground state \(|G_0\rangle\) but in practice this is difficult, and thus the initial state is likely to be a thermal ensemble

\[
\rho(0) = e^{-H_0/k_BT}T, \quad (11)
\]

where \(T\) is temperature and \(k_B\) is the Boltzmann constant, which contains some contribution of the excited states, including states outside the subspace \(\mathcal{H}_{N/2}\). To assess the effectiveness of the optimal control pulse generated for the ground state in this case, we evolve the initial state \(|\Pi\rangle\) under the action of the total Hamiltonian \(H(t)\) given in Eq. (5) subject to

\[
\rho(t_f) = \exp_+ \left[ -i \int_0^{t_f} H(t) dt \right] \rho(0) \exp_+ \left[ -i \int_0^{t_f} H(t) dt \right] \equiv \rho(t_f), \quad (12)
\]

where \(\rho(t_f)\) indicates positive time ordering, and compute the density matrix for the end spins \(\rho_{1N}(t_f)\) by tracing out the interior spins. Fig. 3 shows the resulting entanglement as measured by the concurrence as a function of \(k_BT\). For sufficiently low temperatures \(T\) the optimal control field still generates good entanglement. For example, for a chain of length \(N = 10\) entanglement survives up to \(k_BT/J \approx 1.2\). Moreover, Fig. 3 shows that for low temperatures the concurrence is rather flat, implying that up to a certain temperature the control performance is minimally affected by thermalization. The width of the plateau is related to the energy gap between the ground state and the first excited state. For thermal energies \(k_BT\) less than this energy gap the population of the excited states remains very small, and only when \(k_BT\) exceeds this limit other eigenstates become populated. Since the energy gap between the ground state and first excited states decreases with chain length, the width of the plateau also decreases.

These results are consistent with expectations. For low temperatures the ground state of the system dominates the mixture of the thermal state \(|\Pi\rangle\), and the optimal control pulse transfers this to a \(+1\)-eigenstate of \(A\) that has unit concurrence. Most of the other states of the initial ensemble will be mapped to \(0\)-eigenstates of \(A\) and not contribute to the entanglement between the end spins, but if the initial populations of the excited states are small, the pulse will remain mostly effective. The results can be improved greatly if we calculate the optimal pulse for the initial thermal state, rather than us-
FIG. 4: (Color online) (a) Optimal control pulse $B_c(t)$ obtained by optimizing $\text{Tr}[\rho(t_f)]$ for an initial thermal ensemble with $k_BT/J = 2$ for $N = 4$. (b) If this pulse is applied to initial ensembles $\rho(0)$ with $k_BT/J$ ranging from 0 to 2, the fidelity $\text{Tr}[\rho(t_f)]$ achieved (squares) assumes its theoretical upper bound (solid blue line), showing that this field is optimal in terms of maximizing $\text{Tr}[\rho(t_f)]$ for initial ensembles over a wide range of temperatures. Accordingly, the corresponding entanglement as measured by the concurrence of the reduced density matrix $\rho_{12}(t_f)$ for the ensemble-optimized pulse (dashed red line with diamonds) is substantially higher than that for a ground state optimized pulse (green dash-dotted line with circles).

where we have ordered the spectrum and the corresponding eigenstates in an non-increasing way for both $\rho(t_f)$ and $A$. Different thermal ensembles at different temperature have different spectra $w_{n,m}$. However, to realize the upper bound (13), any optimal pulse for a given thermal ensemble must map all the eigenstates $|e_{n,m}\rangle$ to the eigenstates of $A$ in the same order, independent of the actual value of $w_{n,m}$. Therefore, the optimal pulse for a thermal ensemble with $T_1 > 0$ is also an optimal pulse for any thermal ensemble with $T_2 < T_1$, and in particular, it is an optimal pulse for the initial ground state. But the inverse is not true: the optimal pulse obtained if we start in the ground state is in general not optimal for an initial thermal ensemble. This is because the optimal field starting in the ground state is only guaranteed to map the final state onto one of the +1-eigenstates of $A$, but it generally will not map the correct excited states onto other +1-eigenstates of $A$, and therefore it is not an optimal pulse for an initial thermal ensemble. This is illustrated in Fig. 4 which shows that the fidelity that can be achieved if a ground-state optimized pulse is applied to a thermal ensemble with $T > 0$ is strictly smaller than the optimal fidelity that is achievable with a pulse optimized for this thermal ensemble. The concurrence exhibits a similar behavior. For $N = 4$ the final concurrence between the end spins for $k_BT/J = 1$ is 0.9762 vs less than 0.7 for the ground-state optimized pulse in Fig. 5.

### B. Local control with Gaussian leakage

Another central assumption of our control scheme is that the control field is confined and interacts only with the first spin. In practice such perfect confinement is difficult to achieve and any local magnetic field will also affects neighboring spins, although the effect will usually decay with increasing distance from the control spin, the first spin in our case, either exponentially or following a power law.

To assess the effect of leakage on the performance of the control scheme we take the pulses optimized under ideal assumptions and consider what happens if the field decays exponentially with distance thus affecting not only the target spin but also neighboring spins, effectively changing the control Hamiltonian to

$$H_c = B(t)\hat{H}_1 = B(t)\sum_{k=1}^{N} e^{-(k-1)/\xi}Z_k \tag{15}$$

where $\xi$ is a parameter quantifying the field leakage with $\xi = 0$ corresponding to the ideal case where the field is completely localized and affects only the first spin. Leakage increases with $\xi$ and for $\xi \to \infty$ the control field is uniform, resulting merely in a dynamic global energy shift or global phase. Fig. 5 shows the effect of leakage on the entanglement between the end spins at the final time as a function of the parameter $\xi$. As expected, entanglement decays with increasing $\xi$ but even for $10\%$ leakage we still have a good entanglement. Furthermore, if the leakage parameter $\xi$ is approximately known, we can again incorporate this information into
the optimization, replacing $H_1$ by $\tilde{H}_1$ and then doing the optimization. This substantially improves the results, allowing us to achieve consistently high entanglement for a wide range of $\xi$, although for very large $\xi$ $H_1$ almost commutes with $H_0$, rendering the control increasingly ineffective (see Fig. 5).

C. Random Couplings

Another assumption in our model-based optimal control scheme is that the system Hamiltonian $H_0$ is homogeneous and known. In practice, there is no guarantee that the Hamiltonian of the system will be this perfect. In particular the $J$-couplings between neighboring spins are likely to be subject to random variations and the precise actual values of the couplings may not be known, leading to an uncertainty in the system Hamiltonian. It is therefore very important to consider how small random variations of the coupling strengths are likely to affect the effectiveness of the control scheme. To this end, let us assume that the coupling between neighboring sites are random and vary around an average value $J$, leading to an actual system Hamiltonian of the form

$$H_s = J \tilde{H}_0 = J \sum_{n=1}^{N-1} (1+\epsilon_n) (X_n X_{n+1} + Y_n Y_{n+1} + Z_n Z_{n+1}),$$

(16)

where $\epsilon_n \in [-\alpha, +\alpha]$ is a uniformly distributed random variable with mean 0. Assuming that the precise actual couplings are not known, the best we can do is to study the average effect of random variations of the coupling strengths of a certain magnitude $\alpha$ on the entanglement generated. To this end, we evolve the ground state of the (randomly) perturbed Hamiltonian (16) according to the Schrödinger equation with $H = JH_0 + B(t)H_1$ with $B(t)$ being the pulse optimized for the ideal Hamiltonian $H_0$ and its ground state $|\psi_0\rangle$. The resulting entanglement between the end spins will usually be less than in the ideal case. For comparison we generate 100 different random Hamiltonians $H_0$ for each value of $\alpha$, compute the entanglement attained between the end spins as quantified by the concurrence $C_{1N}$ if we apply the optimal pulse for the ideal case, and take the average $\langle C_{1N} \rangle$.

Fig. 6 shows the average entanglement as a function of $\alpha$. Although the average entanglement decreases with $\alpha$, it remains high for variations up to $\alpha = 0.01J$, showing that a small amount of uncertainty can be tolerated. Larger uncertainties in the coupling strength can be addressed by experimentation or Bayesian estimation techniques [27], and the figure shows that it is highly beneficial to experimentally characterize the couplings to reasonable accuracy, or alternatively, to use adaptive closed-loop experiments [11] to refine the results as disorder or inhomogeneity is not a limiting factor in the optimization per se. If the coupling constants used in the optimization are sufficiently close to the actual couplings, near perfect entanglement can be achieved even for inhomogeneous systems.

FIG. 5: (Color online) Entanglement as a function of leakage $\xi$ for different chain length ($N = 6$ black triangles, $N = 8$ blue squares, $N = 10$ red circles). Solid lines indicate the concurrence dependence for pulses optimized assuming ideal $H_1$ and dashed lines indicate concurrence behavior for pulses optimized with leakage taken into account, i.e., $\tilde{H}_1$. For $\xi$ small the optimal pulses obtained assuming no leakage still achieve high concurrence but if $\xi$ can be estimated, the entanglement generated can be substantially improved by taking leakage into account in the optimization. The inset shows that the optimal pulses in the presence of leakage can differ substantially from the optimal pulses in the absence of leakage. Note that optimal control solutions are not unique and the robustness of individual solutions with regard to leakage varies.

FIG. 6: (Color online) Average entanglement, $\langle C_{1N} \rangle$, in terms of disorder parameter $\alpha$ for different lengths. Each point is the average entanglement over 100 different randomly perturbed Hamiltonians. A small amount of uncertainty in the coupling constants hardly affects the entanglement achieved but for larger variations the entanglement drops significantly. The average entanglement achieved for disordered systems when the actual couplings are used in the optimization (solid black line with triangles for $N = 6$) is very close to one even for high disordered systems, showing that inhomogeneity is not a limiting factor provided the actual couplings can be estimated with sufficient accuracy.
Another interesting feature of Fig. 6 is the fact that longer chains are less sensitive to the random couplings, and thus do not need to be characterized with the same accuracy necessary for shorter chains to obtain the same amount of entanglement. This can be explained in terms of fundamental mathematical properties and the central limit theorem [28], which asserts that when $N$ identical random variables are added, the distribution of the result is Gaussian and its mean and standard deviation are normalized by $N$ and $1/\sqrt{N}$ respectively. This means that the randomness of the system Hamiltonian (16) is effectively suppressed by a factor of $\sqrt{N}$ with increasing $N$.

### D. Decoherence

Another source of errors is from decoherence and population relaxation induced by incoherent interactions of the system with the environment. On the short time scales considered here we expect decoherence due to pure dephasing to be the dominant effect and the system evolution to be governed by a master equation of Lindblad form

$$\dot{\rho} = -i[H(t), \rho] + \mathcal{L}(\rho). \quad (17)$$

To assess how such environmentally induced phase relaxation affects the performance of the optimal control scheme, we compute the evolution of the system according to (17) starting with the initial state $\rho_0 = |G_0\rangle\langle G_0|$, subject to the Hamiltonian $H(t) = JH_0 + B(t)H_1$ as in (3), where $B(t)$ is the optimal pulse for the ideal system, and again calculate the concurrence between the end spins of the final (mixed) state $\rho(t_f)$.

Assuming that the main source of phase relaxation is from the incoherent interactions with the control and measurement apparatus, we consider two types of phase relaxation described by the Lindblad operators

$$\mathcal{L}_1(\rho) = -\gamma\{2\rho - Z_1\rho Z_1 - Z_N\rho Z_N\}, \quad (18a)$$

$$\mathcal{L}_2(\rho) = -\gamma\sum_{i=1}^{N}\{\rho - Z_i\rho Z_i\}. \quad (18b)$$

In the first scheme dephasing affects only the end spins, which are interacting with the probes, while in the second scheme we assume that all spins are affected by dephasing due to imperfect shielding. The resulting entanglement between the end spins in terms of noise strength $\gamma$ in both dephasing cases is shown in Fig. 7 for a chain of length $N = 6$ and $N = 10$. Decoherence reduces the entanglement but when the noise strength is small enough we are still able to generate entanglement with the pulse optimized for the ground state. When more spins are affected by decoherence as in the second scenario, the entanglement decays faster, and the effect of decoherence increases with chain length, as expected. For the scheme to be effective if all spins are subject to dephasing for a chain of length $N = 10$, the relative decoherence rate $\gamma/J$ should be less than 0.1%, which is consistent with usual quantum information processing requirements. The results can generally be improved somewhat if decoherence is taken into account in the optimization process but there are limitations as coherent control cannot compensate for irreversible effects caused by the Lindblad operators. For $\gamma/J < 1$ we find that the pulses obtained by optimization over the Lindblad dynamics generate almost the same amount of entanglement as those computed assuming Hamiltonian dynamics, and for longer chains improvements seem to be even less although it must noted that there are many solutions to the optimal control problem for Hamiltonian systems that achieve near unit concurrence, and the robustness with regard to decoherence of these pulses may vary. Thus a more extensive global search of the parameter space may yield better results.

### VI. CONCLUSION

We have studied control of anti-ferromagnetic isotropic Heisenberg chains using a single control field such as a magnetic field along a given direction acting on a single site. The intrinsic isotropic Heisenberg Hamiltonian commutes with the total spin operator, implying that the dynamics decomposes into $N + 1$ independent excitation subspaces. Although the control is not sufficient for full controllability of the system as the resulting control Hamiltonian commutes with the total spin operator, and hence each excitation subspace is invariant under the dynamics regardless of the control field applied, we verified that the system is controllable in the largest excitation subspace, which guarantees the existence of a control driving the ground state to a perfect end-to-end entangled state in the subspace. Such control can be generated by transforming the control problem to an optimization problem and deriving the optimal control through standard optimization procedure. More importantly, it was shown that the resulting optimal con-
trol solutions are quite robust with regard to multiple sources of imperfections, including imperfect initial state preparation, incomplete confinement of the local control fields, uncertainly about the couplings between adjacent spins and decoherence due to environmental influences.

Furthermore, the quality of the entanglement achieved can be substantially improved by taking the imperfections into account in the optimization. If we can estimate the amount of leakage of the control field or the actual values of the couplings between adjacent spins using experimental system identification techniques, then such information can be incorporated in the optimization to generate greatly improved optimal pulses. Furthermore, we found that a control pulse that maximizes the entanglement between the end spins starting with a high-temperature thermal ensemble is automatically optimal for lower-temperature initial ensembles, which means that the optimal control scheme is effectively independent of the initial state, provided it is a thermal ensemble. Another interesting observation is that simulations strongly suggest that for our problem controllability on the largest excitation subspace holds not only for the isotropic Heisenberg chain but also for a general XXZ model, which deserves future investigation.

VII. ACKNOWLEDGEMENTS

We gratefully thank Pierre de Fouquieres, Peter Pemberton-Ross and Alastair Kay for valuable discussions. SGS acknowledges funding from EPSRC ARF Grant EP/D07192X/1, the QIPIRC and Hitachi. XW thanks the Cambridge Overseas Trust, Hughes Hall and the Cambridge Philosophical Society for support. AB and SB are supported by the EPSRC. SB is also supported by the QIPIRC (GR/S82176/01), the Royal Society and the Wolfson Foundation.

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