All Possible Coupling Schemes in \textit{XY} Spin Chains for Perfect State Transfer

Yaoxiong Wang and Feng Shuang

Institute of Intelligent Machines, Chinese Academy of Sciences, Hefei, China 230031

Herschel Rabitz

Department of Chemistry, Princeton University, Princeton, NJ 08544

We investigate quantum state transfer in \textit{XY} spin chains and propose a recursive procedure to construct the nonuniform couplings of these chains with arbitrary length to achieve perfect state transfer (PST). We show that this method is capable of finding all possible coupling schemes for PST. These schemes, without external control fields, only involve preengineered couplings but not dynamical control of them, so they can be simply realized experimentally. The analytical solutions provide all information for coupling design.

PACS numbers: 03.67.Hk, 05.50.+q

Quantum information and quantum computation can process lots of tasks which are intractable with classical technologies. Although many schemes such as quantum dots\textsuperscript{1}, ion trap\textsuperscript{2}, NMR\textsuperscript{3} have been discussed extensively, a macroscopic scalable quantum computer still seems to need a channel, often known as quantum wire, to transmit or exchange quantum states between inner parts of the quantum computer. These architectures require to implement a transmission process for an unknown quantum state from one place to another which is often called quantum state transfer. In a seminal paper\textsuperscript{4}, Bose proposed a spin chain model, whose evolution was governed by a reasonable Hamiltonian, and considered the fidelity of state transfer in this model. Similar results were also derived by studying dynamical properties of entanglement transition in Heisenberg \textit{XY} spin chain\textsuperscript{5}. This model, in which two processors are connected through a spin chain as quantum wire, is useful for quantum computation based on Heisenberg interaction\textsuperscript{6} or measurements\textsuperscript{7}.

Although some important and significant results have been found, see for example\textsuperscript{5,8}, all of the available results are just concerned with uniform interaction, i.e. the couplings between any two nearest-neighbor sites are the same. For this case, however, it is shown that when \( N \geq 4 \), where \( N \) is the number of the sites in \textit{XY} chain, PST is impossible\textsuperscript{8}. This drawback of uniform interaction motivates people to find some modified models to achieve "long" distance PST. Some works considered long-range interactions\textsuperscript{9}, and some concentrated on numerical simulations\textsuperscript{10}. One feasible choice is to preengineer the couplings\textsuperscript{8}, i.e. choose special nonuniform couplings to achieve PST, and some specific analytical coupling schemes were found\textsuperscript{8,11,12}. The necessary and sufficient conditions for the couplings of PST, which can provide a criterion to verify the preengineered schemes as well as to find new analytical ones, were derived from a more systematical treatment of this problem\textsuperscript{13} by mirror inversion\textsuperscript{11} and quantum computation. However, all these preengineered schemes are obtained through a "verifiable" but not "constructive" way. Thus, we have not yet got all possible coupling schemes for PST.

In this Letter, we start from the necessary and sufficient conditions of PST. After preselecting the eigenvalues of a \textit{XY} spin chain Hamiltonian, we propose two recursive formulas of the couplings for both even and odd \( N \) cases and prove them by mathematical induction. Further discussions demonstrate that this method is capable of finding all possible coupling schemes for PST in \textit{XY} chain with arbitrary length. Experimentally, our PST schemes can be realized, for example, by superconducting circuits and quantum bus\textsuperscript{14}, nanoelectromechanical resonator arrays\textsuperscript{15} or cold-atom optical lattice\textsuperscript{16}.

Next, we first review some basic concepts of state transfer protocol using spin chain as the channel\textsuperscript{17}. An unknown qubit, as encoded in site 1, is attached to one end of a spin chain when the chain is initialized to the all spin-down ground state (state initialization is not necessary\textsuperscript{18}, and our results can be generalized to these cases). Due to the coupling between site 1 and 2, free evolution of the system causes the unknown state to distribute among the chain. After a specific interval, we want to recover this unknown state at the opposite end of the chain to achieve state transfer.

A reasonable Hamiltonian for this task is \textit{XY} type Hamiltonian

\[
H = \frac{1}{2} \sum_{i=1}^{N-1} J_i (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) - \frac{1}{2} \sum_{i=1}^{N} B_i (\sigma_i^z - 1),
\]

where \( J_i \) is the coupling strength between sites \( i \) and \( i+1 \), and \( B_i \) is the external static potential, or control field, at site \( i \). \( \sigma^x, \sigma^y, \sigma^z \) are the three Pauli matrices. One important observation is that Hamiltonian\textsuperscript{17} commutates with the total z-spin operator \( \sum_{i=1}^{N} \sigma_i^z \). Thus, \( \sum_{i=1}^{N} \sigma_i^z \) is a conservation, and the evolution of the system in these state transfer cases will just involve the subspace spanned by ground state and \( N \) one-site excited states. By the
Jordan-Wigner transform, which maps $|i\rangle$ to

$$H = \sum_{i=1}^{N-1} J_i (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + \sum_{i=1}^{N} B_i a_i^\dagger a_i,$$

where $a_i$ and $a_i^\dagger$ are fermionic operators. The $XY$ model can be solved exactly. Hamiltonian $H$ describes an $N$-site hopping model subject to nonuniform external fields. Let $|i\rangle$ denote the single excited state at site $i$, Hamiltonian $H$ in a $2^N$-dimensional space will reduce to an $N$-dimensional subspace spanned by $|ii\rangle$. Explicitly,

$$H_N = \begin{pmatrix} B_1 & J_1 & 0 & \cdots & 0 \\ J_1 & B_2 & J_2 & \cdots & 0 \\ 0 & J_2 & B_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & J_{N-1} \\ 0 & 0 & 0 & \cdots & B_N \end{pmatrix}$$

in $|ii\rangle$ basis. The fidelity of this transfer procedure can be expressed as $\langle N | e^{-iH_N^\dagger N \tau} | 1 \rangle$, where $\tau$ is the time interval of the free evolution. The equivalent conditions for PST, i.e., $|\langle N | e^{-iH_N^\dagger N \tau} | 1 \rangle| = 1$, are: (a) the reflection symmetry $B_i = B_{N+1-i}$ and $J_i = J_{N-i}$. (b) after sorting the eigenvalues of $H_N$ in decreasing order, the difference between any two adjacent eigenvalues is an odd number. All schemes discovered before required (a) as part of their protocols and designed the eigenvalues of $H_N$ to be $\{-k, -k+1, \cdots, 0, k\}$ for $2k \in \mathbb{N}$, $\{q(k^2 + k) + (2p + 1)k\}$ for $k = 0, \ldots, N$ or $\{-k, -k+1, \cdots, 0, k\}$ which all satisfy (b). All these coupling schemes are special solutions for PST, and our main result in this Letter is to show how to get all possible couplings for PST in the absence of external fields, i.e., $B_i = 0$. Because of the perfect transfer condition (a) and the postulation $B_i = 0$, Hamiltonian becomes

$$H_N = \begin{pmatrix} 0 & J_1 & 0 & \cdots & 0 \\ J_1 & 0 & J_2 & \cdots & 0 \\ 0 & J_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & J_2 & 0 \\ 0 & 0 & 0 & 0 & J_1 \end{pmatrix}$$

whose eigenvalues are symmetric about zero. Owing to this symmetry, there are only $[N/2]$ independent couplings and $[N/2]$ independent eigenvalues. (0 is always an eigenvalue when $N$ is odd). Our purpose is to construct the couplings $\{J_i\}$ from a set of preselected eigenvalues $\{\Lambda_i\}$ satisfy (b). We will first consider even $N$ cases and show how to derive $\{J_i\}$ effectively. Then, we generalize these results to odd $N$ cases, and finally show the completeness of this method, i.e. it can get all possible coupling schemes for PST.

For even $N$ cases, we assume the eigenvalues of $H_N$ are $\{\pm \Lambda_1, \ldots, \pm \Lambda_n\}$ where $n = N/2$, $\Lambda_i \in \mathbb{N}$ and $\Lambda_1 > \Lambda_2 > \cdots > \Lambda_n > 0$ (if none of $\{J_i\}$ is zero, then the eigenvalues of $H_N$ are nondegenerate), and omit the scale factor $\pi$. $\{J_i\}$ and $\{\Lambda_i\}$ are connected through the characteristic polynomial of the Hamiltonian $H$:

$$\text{Det}(H_N - \lambda I) = \prod_{i=1}^{n} (\lambda^2 - \Lambda_i^2)$$

which, by expanding it with respect to $\lambda^2$, is equivalent to a set of equations:

$$\sum_{i=1}^{N-1} J_i^2 = \sum_{i=1}^{n} \Lambda_i^2$$

$$\sum_{k_{i+1} - k_i \geq 2} J_{k_{i+1}} J_{k_i} = \sum_{k_{i+1} > k_i} \Lambda_{k_{i+1}}^2 \Lambda_{k_i}^2$$

and we want to derive $\{J_i\}$ from $\{\Lambda_i\}$. This is often called an inverse problem. Notice that we still use $J_{N-i}$ rather than $J_i$ when $i \leq N/2$ despite they are equal just for ease of the expressions. We first introduce some notations for convenience. Denote $j_n^{[N]} = \tau_n N$ and $j_i^{[N]} = (j_i^{[N]})^2$ for $1 \leq i \leq n - 1$. Our meaning will become clear soon. Here, the superscript $N$ denotes the dimension of the matrix $H_N$ and we imply the eigenvalues of $H_D$ are $\{\pm \Lambda_1, \ldots, \pm \Lambda_{D/2}\}$ and its couplings are $\{\xi_i^{[D]}\}$. The main idea is to obtain $\{\xi_i^{[D]}\}$ from $\{\xi_i^{[D-2]}\}$ when we require the Hamiltonians construct by them respectively share the same eigenvalues $\{\pm \Lambda_1, \ldots, \pm \Lambda_{(D-2)/2}\}$. Further, denote $\tau_k = \frac{j_k^{[N]} - j_{k-1}^{[N]} - j_{k+1}^{[N]}}{j_k^{[N]} - j_{k-1}^{[N]} - j_{k+1}^{[N]}}$ for $1 \leq k < n$, where $j_0^{[D]} = 0$ and

$$\Gamma_n^{[N]} = \frac{j_{n-1}^{[N]} - j_{n-2}^{[N]} - j_{n+1}^{[N]}}{j_{n-1}^{[N]} - j_{n-2}^{[N]} - j_{n+1}^{[N]}}$$

and $\Delta_n^{[N]} = j_{n-1}^{[N]}$, $\Delta_n^{[N]} = 1$ where the products in the numerators and denominators involve terms only if the indices of them are not larger than $n - 1$ and $n$ respectively. With these notations, we will show the following equation permits us to get $\{J_i\}$ from $\{\Lambda_i\}$ directly:

$$j_i^{[N]} = \Gamma_i^{[N]} - (-1)^i \Delta_i^{[N]} \Lambda_i^{[N]} \quad i = 1, \ldots, n.$$  

Eq. (7) allows to construct $j_i^{[N]}$ from $\{j_{n-1}^{[N-2]}, \ldots, j_{n-2}^{[N-2]}\}$, $\{j_{n-1}^{[N]}, \ldots, j_{n+1}^{[N]}\}$ and $\Lambda_n$. Thus, when we know $\{j_i^{[N-2]}\}$, by adding one more parameter $\Lambda_n$, we can derive $j_n^{[N]}, j_{n-1}^{[N]} \cdots j_1^{[N]}$ one by one explicitly. Now, we need...
to prove Eq. (7) is consistent with Eq. (6). Direct calculation shows $\Lambda_n$ satisfies a continued fraction:

$$\frac{[N]_{j_n}}{j_{n-1} \cdots j_1 + (-1)^{n-1} \Lambda_n} = 1. \quad (8)$$

$$\frac{[N]_{j_n}}{j_{n-1} \cdots j_1 + (-1)^{n-1} \Lambda_n} + \Lambda_n$$

Eq. (8) is equivalent to $\text{Det}(H_N - \Lambda_n I) = 0$. Actually, by expanding $\text{Det}(H_i - \Lambda I)$ in terms of order $i - 1$ determinants, we will find the original continued fraction for $\text{Det}(H_N - \Lambda_n I) = 0$ is

$$\frac{[N]_{j_n}}{j_{n-1} \cdots j_1 + (-1)^N \Lambda_n} = 0. \quad (9)$$

Due to the symmetry between $J_i$ and $J_{N-i}$, we can move upper half of the continued fraction to the right hand of the equal sign. After taking a square root on both sides, we obtain Eq. (5), which means $\Lambda_n$ is actually an eigenvalue of (4). The square root operation is exactly the origin of why we denote $j_{n} = j_{n}^{[N]}$ but $j_{n}^{[N]} = (j_{n}^{[N]})^2$ for $i \neq n$ before. Next, we will prove Eq. (7) is correct for arbitrary $N$ by mathematical induction. We assume the permutations of $\{\Lambda_1, \Lambda_2, \ldots, (-1)^n \Lambda_{n-1}\}$ form a group keeps $\{j_{i}^{[N-2]}\}$ unchanged which is actually true for $\{j_{2}^{[N]}\}$. The following step is to prove $\{j_{i}^{[N]}\}$ are also invariant under the permutation of $\Lambda_n$ and $-\Lambda_{n-1}$ which, with the assumption above, directly induces $\{\pm \Lambda_i\}$ for $i = 1, \ldots, n$ are the eigenvalues of $H_N$ when $\{j_{i}^{[N]}\}$ are constructed from Eq. (7). Obviously, $j_{n}^{[N]}$ is unchanged under the permutation of $\Lambda_n$ and $-\Lambda_{n-1}$. For $j_{n-1}^{[N]}$, we can expand it using $\Lambda_n$, $\Lambda_{n-1}$ and $\{j_{i}^{[N-4]}\}$ in which $\{j_{i}^{[N-4]}\}$ are irrelevant to $\Lambda_n$ and $\Lambda_{n-1}$. Notice that this expression has similar form with $j_{n-5}^{[N-2]}$ when $j_{n-5}^{[N-2]}$ is expanded by $\Lambda_{n-1}$, $\Lambda_{n-2}$ and $\{j_{i}^{[N-6]}\}$, and if we replace $\Lambda_n$, $\Lambda_{n-1}$ and $\{j_{i}^{[N-4]}\}$ in $j_{n-1}^{[N-4]}$ by $-\Lambda_{n-1}$, $-\Lambda_{n-2}$ and $\{j_{i}^{[N-6]}\}$ respectively, we will find they are indeed the same one. Owing to the assumption that the permutation of $\Lambda_{n-1}$ and $-\Lambda_{n-2}$ keeps $j_{n-5}^{[N-2]}$ unchanged, we conclude that $j_{n-5}^{[N-2]}$ is also unchanged under the permutation of $\Lambda_n$ and $-\Lambda_{n-1}$. This method, demonstrating the invariance by replacement, is applicable for other $j_{i}^{[N]}$, and we can further prove all $\{j_{i}^{[N]}\}$ are invariant under the permutation of $\Lambda_n$ and $-\Lambda_{n-1}$.

Combining this proof and the fact that $\{\Lambda_1, \Lambda_2\}$ actually form a group for $\{j_{1}^{[4]}\}$, we can prove the permutations of $\{\Lambda_1, \Lambda_2, \ldots, (-1)^{n+1} \Lambda_{n}\}$ form a group keeps $\{j_{i}^{[N]}\}$ unchanged. Furthermore, if $\Lambda_n$ is an eigenvalue of (4), then, according to Eq. (5), $\{\pm \Lambda_i\}$ for $i = 1, \ldots, n$ are all eigenvalues of (4). Fig. (1) shows idea of the proof.

For odd $N$ cases, we assume $\Lambda_n > \Lambda_{n-1} > \ldots > \Lambda_1 > 0$. Define $j_{n}^{[N]} = 2(j_{n}^{[N]})^2$ and $j_{n}^{[N]} = (j_{n}^{[N]})^2$ for $1 \leq i \leq n-1$, $n = (N-1)/2$, and define $\Gamma_k$ and $\Delta_k$ as the same as even $N$ cases. The corresponding recursive formula for odd $N$ is

$$j_{k}^{[N]} = \Lambda_k \Delta_k - \Gamma_k$$

$$j_{k-1}^{[N]} = \Delta_k - \Gamma_{k-1}$$

where $k = n, n-2, n-4, \ldots$ till we get $j_1^{[N]}$. The difference between $n$ and $k$ in Eq. (10a) is an even number which implies $\Lambda_k^2$ appears in the right hand of Eq. (10) alternately. Just like even $N$ cases, we can directly check $\Lambda_k$ is an eigenvalue of (4) by the continued fraction representation when $\{J_i\}$ are expressed by Eq. (11), and the factor 2 appears in the definition of $j_{i}^{[N]}$ also comes from the continued fraction structure. Although the main idea is the same, there are still some differences between even and odd cases. First, $\{j_{i}^{[N]}\}$ are no longer unchanged under the permutation of $\Lambda_n$ and $-\Lambda_n$ when $N$ is odd. Instead, the permutations of $\{\Lambda_n, \Lambda_{n-2}, \Lambda_{n-4}, \ldots\}$ and $\{\Lambda_{n-1}, \Lambda_{n-3}, \Lambda_{n-5}, \ldots\}$ form two groups keep $\{j_{i}^{[N]}\}$ invariant respectively (if we consider all the eigenvalues $\{\pm \Lambda_i\}$, then both even and odd cases have two groups formed by interlaced eigenvalues respectively which keep $\{j_{i}^{[N]}\}$ unchanged, see Fig. (1)). Second, it’s interesting to see $\frac{[N]_{j_n}}{j_{n-1} \cdots j_1 + (-1)^{N-1} \Lambda_{n-1}}$ and $\frac{[N]_{j_n}}{j_{n-1} \cdots j_1 + (-1)^{N-2} \Lambda_{n-2}}$ have the same structure when a similar replacement as in even $N$ cases has been made. With the help of this property, we can prove $\Lambda_{n-1}$ is also an eigenvalue of $H_n$. Combining it with the fact that $\Lambda_n$ is an eigenvalue of $H_N$ and the symmetry property between $\Lambda_n$ and $\Lambda_{n-2}$, by means of mathematical induction, we assert the eigenvalues of $H_N$ whose off-diagonal elements are constructed from Eq. (10) are

![Figure 1](image-url)
The completeness of this method comes from the fact that \( J_i \) is uniquely determined by its eigenvalues when \( \{ J_i \} \) are all positive \([20]\). This also implies all real coupling schemes for \( J_i \) are uniquely determined by its eigenvalues. Since the completeness is available only if all \( \{ J_i \} \) are real, we need to prove the positivity of \( \{ J_i \} \) for Eq.(7) and Eq.(10). This is more apparent when we factor out the common factors of each equation in Eq.(7) and Eq.(10). After factorization, we will find each expression contains two factors, one is positive and the other is monotone with respect to \( \Lambda \). Considering \( \Lambda_{n-1} > \Lambda_n > 0 \) and \( \Lambda_n > \Lambda_{n-1} \) in even and odd cases respectively, we assert \( \{\Lambda_{n-1}^{(N)}\} \) are all positive and \( \{ J_i \} \) are all real which satisfy the completeness condition. In a word, Eq.(7) and Eq.(10) are complete for all possible coupling schemes.

Up to now, we have solved both even and odd \( N \) cases in the absence of external control fields \( \{ B_i \} \). This constructive method allows us to calculate the couplings from a set of preselected eigenvalues. We have chosen several sets of 50 numbers whose interval between any two adjacent ones in each set is a random odd number in the domain \([1, 100]\). In general, we got the couplings within 10 seconds. This numerical calculation shows our method is effective. Although the resultant couplings often have enormous numerators and denominators caused by the continued fraction structure of the constructive method, we can choose some specific eigenvalues and then get compact coupling schemes. For example, choosing the eigenvalues as \( \{\pm(T + \frac{i}{2} + i(2S + 1))\} \), where \( T \) and \( S \) are two non-negative integers, for \( i = 1, 2, \ldots, \frac{N}{2} \) when \( N \) is even, we will find \( J_i^2 \) are \( \frac{((N-1)(1+2S)+4}{4} \) and \( \frac{(1+2T+1+i)(1+2S)(1+2T+1+i)(1+2S)}{(1+2T)(1+2S)(1+2T+1+i)(1+2S)} \) for even and odd \( i \) respectively.

The model used here is also similar to that we encounter in population transfer in an \( N \)-level system in which \( N \) discrete energy levels are equivalent to \( N \) single excited states \( \{|i\} \). Assuming the only interaction to be that of electric-dipole transitions and each frequency of the laser to be close to resonance with two adjacent states, after rotating wave approximation (a general review of this topic, see \([21]\)), Hamiltonian of this problem is identical to Eq.(1) when we treat the dipole interactions as the couplings in \( XY \) chain. Our results for PST can also be used to design the amplitude of each frequency of the control laser to achieve perfect population transfer.

In this Letter, we have considered the problem of transferring an unknown state from one end of a spin chain to the other end, and proposed two recursive formulas for designing the couplings since uniform coupled \( XY \) chains can not afford PST. We also prove these formulas are complete. Although this method is numerically effective, there are still some interesting issues. We set the diagonal elements to be zeros, i.e. there is no external control field in spin chain or the laser resonances with any two adjacent levels in an \( N \)-level system. This is not necessary for PST or perfect population transfer. Non-zero diagonal elements break the symmetry of the spectrum of the Hamiltonian, and the eigenvalues no longer appear in pairs. Nevertheless, the continued fraction is also available when we replace \( \Lambda \) by \( B_i - \Lambda \). We expect similar formula for cases involve control fields which, of course, will contain \( N \) recursive equations but not \( \lfloor N/2 \rfloor \) for an \( N \)-site spin chain. Another question is whether there are other similar coupling schemes for special selected eigenvalues. We have tested some simple sets of eigenvalues, but the couplings still seem complicated.

This work was supported in part by Foundation of President of Hefei Institutes of Physical Science CAS, one of us (F.S.) was also partly supported by National Natural Science Foundation of China (No. 61074052).

References:
[1] D. Loss and D. DiVincenzo, Phys. Rev. A 57, 120 (1998).
[2] J. Cirac and P. Zoller, Phys. Rev. Lett. 74, 4091 (1995).
[3] D. Cory et al., Proc. Natl. Acad. Sci. 94, 1634 (1997).
[4] S. Bose, Phys. Rev. Lett. 91, 207901 (2003).
[5] V. Subrahmanyan, Phys. Rev. A 69, 034304 (2004).
[6] D. DiVincenzo et al., Nature 408, 339 (2000).
[7] R. Raussendorf and H. Briegel, Phys. Rev. Lett. 86, 5188 (2001); R. Raussendorf et al., Phys. Rev. A 68, 022312 (2003).
[8] M. Christandl et al., Phys. Rev. Lett. 92, 187902 (2004); M. Christandl et al., Phys. Rev. A 71, 032312 (2005).
[9] A. Kay, Phys. Rev. A 73, 032306 (2006); G. Gualdi et al., Phys. Rev. A 78, 022325 (2008).
[10] P. Karbach and J. Stolze, Phys. Rev. A 72, 030301 (2005); A. Wójcik et al., Phys. Rev. A 72, 034303 (2005).
[11] C. Albanese et al., Phys. Rev. Lett. 93, 230502 (2004).
[12] C. Shi et al., Phys. Rev. A 71, 032309 (2005).
[13] M.-H. Yung and S. Bose, Phys. Rev. A 71, 032310 (2005).
[14] J. Q. You and F. Nori, Phys. Today 58, 42 (2005); J. Majer et al., Nature 449, 443 (2007).
[15] P. Rabl, et al., Nat. Phys. 6, 602 (2010).
[16] I. Bloch, Nature 453, 1016 (2008).
[17] S. Bose, Contemporary Physics 48, 13 (2007); A. Kay, Int. J. Quan. Info. 8, 641 (2010).
[18] C. Di Franco et al., Phys. Rev. Lett. 101, 230502 (2008).
[19] J. Wilkinson, The Algebraic eigenvalue problem (Clarendon Press, 1965).
[20] H. Hochstadt, Linear Algebra and Its Applications 8, 435 (1974).
[21] B. Shore, Acta Physica Slovaca 58, 243 (2008).