All possible coupling schemes in XY spin chains for perfect state transfer

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We investigate quantum state transfer in XY spin chains and propose a recursive procedure to construct the nonuniform couplings within these chains of arbitrary length in order to achieve perfect state transfer. We show that this method is capable of finding all possible coupling schemes for perfect state transfer. These schemes, without external control fields, involve analytically identified engineered couplings without the need for dynamical control. The analytical solutions provide all information for coupling design.

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I. INTRODUCTION

Quantum computation allows to address tasks which are intractable with classical technologies. Many schemes have been proposed to realize quantum computation [1] and a quantum computer will likely need a channel, often known as a quantum wire, to transmit or exchange quantum states between the components of the machine. The latter objective calls for implementing the transmission of an unknown quantum state from one place to another, which is often referred to as quantum state transfer. In a seminal paper [2], Bose proposed a spin chain model for this purpose and considered the fidelity of state transfer. Similar results were also derived from studying the dynamical properties of entanglement in Heisenberg XY spin chains [3]. This model, in which two processors are connected through a spin chain as quantum wire, is useful for quantum computation based on Heisenberg interactions [4] or special measurements [5].

Although some important and significant results have been found for state transfer (see for example [2,3]), all of the prior studies are concerned with uniform interactions; i.e., the couplings between all nearest-neighbor sites are the same. Under this restriction, however, it was shown that when $N \geqslant 4$ (where N is the number of the sites in the XY chain), perfect state transfer (PST) is not possible [6]. This drawback of a uniform interaction has motivated efforts to find modified models for achieving "long"-distance PST. Some works considered long-range interactions [7] and explored some numerical properties of PST [8]. Another route is to engineer the couplings [6] (i.e., create special nonuniform couplings to achieve PST), and some specific analytically identified coupling schemes were found [6,9,10]. The necessary and sufficient conditions for the PST couplings were derived from a systematic treatment of the problem [11] by mirror inversion [9] and computational treatment. However, all these analytical engineered schemes are based on verification and do not present a constructive means to find the couplings. Thus, these prior works have left wanting the means to get all possible coupling schemes for PST.

In this paper, we start from the necessary and sufficient conditions of PST. After preselecting the eigenvalues of an XY spin chain Hamiltonian, we propose two recursive formulas to determine the couplings for both even and odd N cases and prove the validity of the scheme by mathematical induction. We demonstrate that this method is capable of finding all possible coupling schemes for PST in an XY chain of arbitrary length. Experimentally, the resultant PST schemes could be realized, for example, by superconducting circuits and quantum buses [12], nanoelectromechanical resonator arrays [13], or cold-atom optical lattices [14].

II. SPIN CHAIN FOR STATE TRANSFER

We first review some basic concepts of the state transfer protocol using a spin chain as the channel [2,15]. An unknown qubit, as encoded in site 1, is attached to one end of a spin chain with the chain initialized to the all spin-down ground state. In practice, however, state initialization is not necessary for some spin chain models [16]. Due to the coupling between the spins of the chain, free evolution of the system causes the unknown state to distribute along the chain. After a specific interval, the goal is to recover this unknown state at the opposite end of the chain and thereby achieve state transfer.

A reasonable Hamiltonian for this task is of the XY form

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

where J_i is the coupling strength between sites i and $i+1$, and B_i is the external control field at site i. σ^x, σ^y, and σ^z are the three Pauli matrices. Since the Hamiltonian (1) commutates with the total z-spin operator $\sum_{i=1}^{N}\sigma_i^z$, the evolution of the system will just involve the subspace spanned by the ground state and N one-site excited states. By the Jordan-Wigner transform, the Hamiltonian in (1) can be mapped to

$$H = \sum_{i=1}^{N-1} J_i(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + \sum_{i=1}^{N} B_i a_i^\dagger a_i, \quad (2)$$

which presents an exactly solvable model. Hamiltonian (2) describes an N-site hopping model with nonuniform external fields. Let $|i\rangle$ denote the single excited state at site i, then the Hamiltonian (2) can be expressed in the N-dimensional

subspace spanned by $\{|i\rangle\}$,

$$H_N = \begin{pmatrix} B_1 & J_1 & 0 & \cdots & 0 \\ J_1 & B_2 & J_2 & \cdots & 0 \\ 0 & J_2 & B_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & J_{N-1} \\ 0 & 0 & 0 & J_{N-1} & B_N \end{pmatrix}. \tag{3}$$

The fidelity of this transfer process is $|\langle N|e^{-iH_N\tau}|1\rangle|$, where τ is the time interval of the evolution. The conditions for PST, i.e., $|\langle N|e^{-iH_N\tau}|1\rangle| = 1$, are (a) reflection symmetry $B_i = B_{N+1-i}$ and $J_i = J_{N-i}$ and (b) after sorting the eigenvalues of $H_N\frac{\tau}{\pi}$ in decreasing order, the difference between any two adjacent eigenvalues must be an odd integer [11]. All prior schemes required (a) as part of their protocols and designated the eigenvalues of $H_N\frac{\tau}{\pi}$ to be $\{-k, -k+1, \ldots, k-1, k\}$ for $2k \in \mathbb{N}$ [6,9], $\{q(k^2+k)+(2p+1)k\}$ for $k = 0, \ldots, N$ [9], or $\{-k+\frac{1}{2}-n, \ldots, -k-\frac{3}{2}, -k-\frac{1}{2}, k+\frac{1}{2}, k+\frac{3}{2}, \ldots, k-\frac{1}{2}+n\}$ [10], which all satisfy (b).

III. ALL POSSIBLE COUPLING SCHEMES FOR PST WITHOUT CONTROL FIELDS

All of the coupling schemes listed above are particular solutions for PST, and the main result of this paper is to attain all possible couplings for PST in the absence of external fields, i.e., $B_i = 0$; the prospect of fields being present will be discussed at the end of the paper. By utilizing the perfect transfer condition (a) and $B_i = 0$, the Hamiltonian (3) becomes

$$H_N = \begin{pmatrix} 0 & J_1 & 0 & \cdots & 0 & 0 \\ J_1 & 0 & J_2 & \cdots & 0 & 0 \\ 0 & J_2 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & J_2 & 0 \\ 0 & 0 & 0 & J_2 & 0 & J_1 \\ 0 & 0 & 0 & 0 & J_1 & 0 \end{pmatrix}, \tag{4}$$

whose eigenvalues are symmetric about zero. Owing to this symmetry, there are only $\frac{N}{2}$ ($\frac{N-1}{2}$) independent couplings and $\frac{N}{2}$ ($\frac{N-1}{2}$) independent eigenvalues in (4) for even (odd) N cases (0 is always an eigenvalue when N is odd). The goal is to construct the couplings $\{J_i\}$ from a set of preselected eigenvalues $\{\Lambda_i\}$ that satisfy (b). We will first consider even N and show how to derive $\{J_i\}$. Then, these results are generalized to odd N, and we finally show how to attain all possible coupling schemes for PST.

For even N, we write the eigenvalues of H_N as $\{\pm\Lambda_1, \ldots, \pm\Lambda_n\}$, where $n = N/2$, $\Lambda_i \in \mathbb{N}$, and $\Lambda_1 > \Lambda_2 > \cdots > \Lambda_n > 0$ (if none of the $\{J_i\}$ is zero, then the eigenvalues of H_N are nondegenerate [17]), and we omit the scale factor $\frac{\tau}{\pi}$. $\{J_i\}$ and $\{\Lambda_i\}$ are connected through the characteristic polynomial of the Hamiltonian (4),

$$\mathrm{Det}(H_N - \lambda I) = \prod_{i=1}^{n}\left(\lambda^2 - \Lambda_i^2\right), \tag{5}$$

which, by expanding in powers of λ^2, is equivalent to a set of equations

$$\sum_{i=1}^{N-1} J_i^2 = \sum_{i=1}^{n} \Lambda_i^2, \tag{6a}$$

$$\vdots$$

$$\sum_{k_{i+1}-k_i\geqslant 2} J_{k_1}^2 \cdots J_{k_n}^2 = \sum_{k_{i+1}>k_i} \Lambda_{k_1}^2 \cdots \Lambda_{k_n}^2, \tag{6b}$$

$$\vdots$$

$$\prod J_1^2 J_3^2 \cdots J_{N-1}^2 = \prod_{i=1}^{n} \Lambda_i^2. \tag{6c}$$

We want to derive $\{J_i\}$ from $\{\Lambda_i\}$. We retain J_{N-i} rather than J_i when $i \leqslant N/2$ in Eq. (6), despite they being equal, for clarity of the analysis and introduce the following notation for convenience. Denote

$$j_n^{[N]} = J_n^{[N]}, \tag{7a}$$

$$j_i^{[N]} = (J_i^{[N]})^2, \quad 1 \leqslant i \leqslant n-1, \tag{7b}$$

whose meaning will become clear shortly. Here, the superscript N indicates the dimension of the matrix H_N and we imply that the eigenvalues of H_D are $\{\pm\Lambda_1, \ldots, \pm\Lambda_{D/2}\}$ and its couplings are $\{J_i^{[D]}\}$. The main concept underlying the procedure is to obtain $\{j_i^{[D]}\}$ from $\{j_i^{[D-2]}\}$, requiring that the Hamiltonians are constructed to respectively share the same eigenvalues $\{\pm\Lambda_1, \ldots, \pm\Lambda_{(D-2)/2}\}$. Further, we denote

$$\Gamma_k^N = \frac{j_{n-1}^{[N-2]} j_{n-2}^{[N-2]} \cdots j_{k-1}^{[N-2]}}{j_n^{[N]} j_{n-1}^{[N]} \cdots j_{k+1}^{[N]}}, \quad 1 \leqslant k < n, \tag{8a}$$

$$\Delta_k^N = \frac{j_k^{[N-2]} j_{k+2}^{[N-2]} j_{k+4}^{[N-2]} \cdots}{j_{k+2}^{[N]} j_{k+4}^{[N]} j_{k+6}^{[N]} \cdots}, \quad 1 \leqslant k < n-1, \tag{8b}$$

where $j_0^{[D]} \equiv 0$, $\Gamma_n^N = j_{n-1}^{[N-2]}$ and $\Delta_{n-1}^N = j_{n-1}^{[N-2]}$, $\Delta_n^N = 1$. The products in the numerators and denominators of Eq. (8) contain terms with indices no larger than $n-1$ and n, respectively. With this notation, we will show that the following equation allows us to directly attain $\{J_i\}$ from $\{\Lambda_i\}$:

$$j_i^{[N]} = \Gamma_i^N - (-1)^i \Lambda_n \Delta_i^N, \quad i = 1, \ldots, n. \tag{9}$$

Equation (9) allows for constructing $j_i^{[N]}$ from $\{j_{n-1}^{[N-2]}, \ldots, j_{i-1}^{[N-2]}\}$, $\{j_n^{[N]}, \ldots, j_{i+1}^{[N]}\}$, and Λ_n. Thus, when we know $\{j_i^{[N-2]}\}$, by adding one more eigenvalue Λ_n, we can derive $j_n^{[N]}, j_{n-1}^{[N]}, \ldots, j_1^{[N]}$ one by one explicitly. Now, we need to prove Eq. (9) is consistent with Eq. (6). Direct calculation shows that Λ_n satisfies a continued fraction:

$$\cfrac{j_n^{[N]}}{\cfrac{j_{n-1}^{[N]}}{\vdots \; + (-1)^{n-1}\Lambda_n}} = 1. \tag{10}$$

Equation (10) is equivalent to $\mathrm{Det}(H_N - \Lambda_n I) = 0$. By expanding $\mathrm{Det}(H_i - \Lambda I)$ in terms of order $i-1$ determinants, we will find that the original continued fraction for

$\mathrm{Det}(H_N - \Lambda_n I) = 0$ is

$$\cfrac{\left(J_{N-1}^{[N]}\right)^2}{\begin{array}{c}\vdots\\ \cfrac{(J_2^{[N]})^2}{\cfrac{(J_1^{[N]})^2}{\Lambda_n}-\Lambda_n}+\Lambda_n\end{array}} - \Lambda_n + (-1)^{N-1}\Lambda_n = 0. \tag{11}$$

Due to the symmetry between J_i and J_{N-i}, we can move the upper half of the continued fraction to the right-hand side of the equation. After taking a square root on both sides, we obtain Eq. (10), which means that Λ_n is actually an eigenvalue of (4). The square root operation is the origin of why we denoted $j_n^{[N]} = J_n^{[N]}$ but $j_i^{[N]} = (J_i^{[N]})^2$ for $i \neq n$. Next, we will prove that Eq. (9) is valid for arbitrary N by mathematical induction. We assume that permutations of $\{\Lambda_1, -\Lambda_2, \Lambda_3, \ldots, (-1)^n \Lambda_{n-1}\}$ leave $\{j_i^{[N-2]}\}$ invariant, which can be shown to be explicit for $\{j_i^{[4]}\}$. The next step is to prove that the $\{j_i^{[N]}\}$ are also invariant under the permutation of Λ_n and $-\Lambda_{n-1}$, which, with the assumption above, directly implies that $\{\pm\Lambda_i\}$ for $i = 1, \ldots, n$ are the eigenvalues of H_N when $\{J_i^{[N]}\}$ are constructed from Eq. (9). Obviously, $j_n^{[N]}$ is unchanged under the permutation of Λ_n and $-\Lambda_{n-1}$. For $j_{n-1}^{[N]}$, we can expand it using Λ_n, Λ_{n-1}, and $\{j_i^{[N-4]}\}$ in which $\{j_i^{[N-4]}\}$ do not depend on Λ_n and Λ_{n-1}. Note that this expression has a form similar to $j_{n-5}^{[N-2]}$ upon expansion in terms of Λ_{n-1}, Λ_{n-2}, and $\{j_i^{[N-6]}\}$; if we replace Λ_n, Λ_{n-1}, and $\{j_i^{[N-4]}\}$ in $j_{n-1}^{[N]}$ by $-\Lambda_{n-1}$, $-\Lambda_{n-2}$, and $\{j_i^{[N-6]}\}$, respectively, we will find they are indeed equivalent. Owing to the assumption that the permutation of Λ_{n-1} and $-\Lambda_{n-2}$ keeps $j_{n-5}^{[N-2]}$ unchanged, we conclude that $j_{n-1}^{[N]}$ is also unchanged under the permutation of Λ_n and $-\Lambda_{n-1}$. This method is applicable for other $j_i^{[N]}$, and we can further prove that the permutation of Λ_n and $-\Lambda_{n-1}$ leaves all $\{j_i^{[N]}\}$ invariant.

Combining this proof and the fact that permutations of $\{\Lambda_1, -\Lambda_2\}$ form a group which leaves $\{j_1^{[4]}, j_2^{[4]}\}$ invariant, we can prove that the permutations of $\{\Lambda_1, -\Lambda_2, \ldots, (-1)^{n+1}\Lambda_n\}$ form a group that leaves $\{j_i^{[N]}\}$ invariant. Furthermore, if Λ_n is an eigenvalue of (4), then, according to Eq. (10), $\{\pm\Lambda_i\}$ for $i = 1, \ldots, n$ are all eigenvalues of (4). Figure 1 shows a schematic of the proof.

For odd-N cases, we assume $\Lambda_n > \Lambda_{n-1} > \cdots > \Lambda_1 > 0$. Let $n = (N-1)/2$, and define

$$j_n^{[N]} = 2(J_n^{[N]})^2, \tag{12a}$$

$$j_i^{[N]} = \left(J_i^{[N]}\right)^2, \quad 1 \leqslant i \leqslant n-1. \tag{12b}$$

Further, define Γ_k^N and Δ_k^N as the same as even-N cases. The corresponding recursive formula for odd N is

$$j_k^{[N]} = \Lambda_n^2 \Delta_k^N - \Gamma_k^N, \tag{13a}$$

$$j_{k-1}^{[N]} = \Delta_{k-1}^N - \Gamma_{k-1}^N, \tag{13b}$$

where $k = n, n-2, n-4, \ldots$ until we get $j_1^{[N]}$. The difference between n and k in Eq. (13a) is an even integer, which implies that Λ_n^2 appears on the right side of Eq. (13) alternately. Just like the even-N cases, we can directly check that Λ_n is an eigenvalue of (4) by the continued fraction representation when the $\{J_i\}$ are expressed by Eq. (13), and the factor 2 appearing in the definition of $j_n^{[N]}$ also comes from the continued fraction structure. Although the main concept of the proof is the same, there are some differences between even and odd cases. First, the $\{j_i^{[N]}\}$ are no longer unchanged under the permutation of Λ_n and $-\Lambda_{n-1}$ 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 to 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.) Note that $\cfrac{j_3^{[N]}}{\cfrac{j_2^{[N]}}{\cfrac{j_1^{[N]}}{\Lambda_{n-1}}-\Lambda_{n-1}}+\Lambda_{n-1}}$ and $\cfrac{j_2^{[N-2]}}{\cfrac{j_1^{[N-2]}}{\Lambda_{n-2}}-\Lambda_{n-2}}$ have the same structure when a similar replacement is made as in proving the even-N cases. Utilizing this property, we can prove that Λ_{n-1} is also an eigenvalues of H_N. Combined with the fact that Λ_n is an eigenvalue of H_N and the symmetry property between Λ_n and Λ_{n-2}, by means of mathematical induction, we conclude that the eigenvalues of H_N, whose off-diagonal elements are constructed from Eq. (13), are $\{0, \pm\Lambda_i\}$ for $i = 1, \ldots, n$.

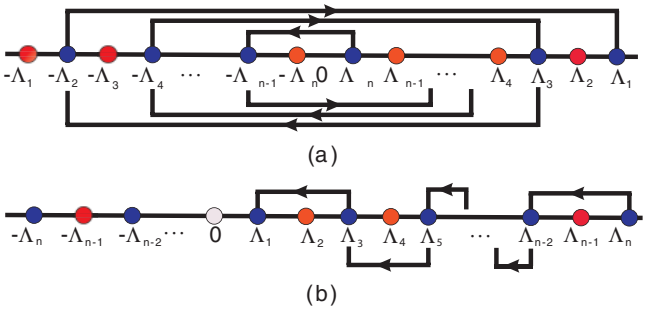

FIG. 1. (Color online) Recursive procedures for (a) even and (b) odd N cases. Permutations of $\{\Lambda_i\}$ with the same color form one group. Although 0 is always an eigenvalue in (b), the permutation group does not contain it. Arrows on the straight lines indicate the recursive directions; e.g., the rightmost arrow in (b) implies that if Λ_n is an eigenvalue of (4) when $\{J_i\}$ are constructed from Eq. (13), then so is Λ_{n-2} an eigenvalue.

The completeness of this method comes from the fact that (3) is uniquely determined by its eigenvalues when the $\{J_i\}$ are all positive [18]. This circumstance also implies that all real coupling schemes for (4) 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 $\{J_i^2\}$ for Eq. (9) and Eq. (13). This is more apparent when we extract the common factors in Eq. (9) and Eq. (13). As a result, we will find that each expression contains two factors, one positive and the other monotonic with respect to Λ_n. Considering $\Lambda_{n-1} > \Lambda_n > 0$ and $\Lambda_n > \Lambda_{n-1}$ in even and odd cases, respectively, we see that the $\{j_n^{[N]}\}$ are all positive and the $\{J_i\}$ are all real, which satisfies the completeness condition. Thus, Eq. (9) and Eq. (13) are complete for all possible coupling schemes.

The constructive method presented here permitted calculating the couplings from a set of preselected eigenvalues. As a numerical test, we chose several sets of 50 eigenvalues whose interval between any two adjacent ones in each set is

a random odd integer in the domain [1,100]. The recursion algorithm was accomplished just on a common PC (2.50 GHz CPU and 2 GB memory) and the running time is generally within 10 s. Following the recursion algorithm readily identified the couplings in the Hamiltonian. The resultant couplings often have large numerators and denominators in the continued fractions, but it is possible to choose specific eigenvalues to avoid this circumstance. For example, choosing the eigenvalues as $\{\pm[T+\frac{1}{2}+i(2S+1)]\}$, where T and S are two non-negative integers, for $i=1,2\ldots,\frac{N}{2}$ when N is even, we will find that the J_i^2 are $\frac{i(N-i)(1+2S)^2}{4}$ and $\frac{[(1+2T)+(1+i)(1+2S)][(1+2T)+(N+1-i)(1+2S)]}{4}$ for even and odd i, respectively.

The model used here is also similar to that encountered in population transfer in an N-level system in which N discrete energy levels are equivalent to N single excited states $\{|i\rangle\}$. In this case, by assuming that the only interaction is electric-dipole coupling and the laser is close to resonance with all adjacent states, then after applying the rotating wave approximation [19], the Hamiltonian of this problem is identical to Eq. (4) when we treat the dipole interactions analogously to the couplings in the XY chain. In this case our results for PST can also be used to design the amplitude of each frequency of the control laser to achieve perfect population transfer.

IV. CONCLUSION

In this paper, we have considered the problem of transferring an unknown state from one end of a spin chain to the other end, and we presented recursive formulas for determining the couplings, since uniform coupled XY chains cannot afford PST. Although this method is numerically effective, there are still some interesting remaining issues. We set the diagonal elements of the Hamiltonian to be zero; i.e., there is no external control field in the spin chain or analogously the laser resonances between adjacent levels in an N-level system. These conditions are not necessary for PST or perfect population transfer. Nonzero diagonal elements break the symmetry of the Hamiltonian spectrum, and the eigenvalues no longer appear in pairs. Nevertheless, the continued fraction approach is also valid when we replace Λ by $B_i-\Lambda$. We expect similar formulas for cases that involve control fields, which will contain N recursive equations for an N-site spin chain.

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