

Pretty Good State Transfer in Qubit Chains - The Heisenberg Hamiltonian

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Pretty good state transfer in networks of qubits occurs when a continuous-time quantum walk allows the transmission of a qubit state from one node of the network to another, with fidelity arbitrarily close to 1. We prove that in a Heisenberg chain with n qubits there is pretty good state transfer between the nodes at the j -th and $(n-j+1)$ -th position if n is prime congruent to 1 modulo 4 or a power of 2. Moreover, this condition is also necessary for $j = 1$. We obtain this result by applying a theorem due to Kronecker about Diophantine approximations, together with techniques from algebraic graph theory.

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I. INTRODUCTION

Long-distance quantum communication, for example over several kilometers, typically uses photonic systems. On the other hand, given the difficulty of engineering interactions between photons, several promising candidates for quantum hardware are based on *quantum networks* of localized qubits¹, which are easier to manipulate. In typical quantum algorithms during the computation the states of different qubits have to be transferred between various registers, namely between different nodes of the network. However, when qubits are localized, their physical movement may be either impossible, by construction, or energy inefficient. A viable solution to this problem is to exploit the coherent dynamics of the quantum network, namely a continuous-time quantum walk, to transfer the quantum states between different nodes². This approach for short-distance (*in-chip*) communication has attracted much attention³ because it minimizes the use of external control and also avoids the complex interface between localized and moving particles. However, in a generic quantum network the resulting coherent dynamics is very complicated and the transmission between two nodes is normally inefficient. Therefore, much effort has been devoted to understand what are the best strategies, or the best networks, to achieve either *perfect state transfer* between distant nodes⁴⁻⁷, or *pretty good state transfer*⁸⁻¹³ where the transmission quality is *almost* perfect. One-dimensional systems, namely chains of qubits, are perhaps the most natural candidate for transmission as they resemble a quantum wire or *data-bus*.

Most of the literature on perfect or pretty good state transfer has considered chains interacting with the XY Hamiltonian because they offer several mathematical simplifications, e.g. the Hamiltonian in the single-particle subspace is equivalent to the adjacency matrix of the corresponding graph and also the many-particle problem is exactly solvable¹⁴. However, in solid state systems such as quantum dots¹⁵ or dopants in silicon¹⁶ and in current optical lattice experiments¹⁷, which are some of the most promising quantum devices, the natural interaction is the Heisenberg (XYZ) Hamiltonian. Motivated by this, in this paper we focus on unmodulated qubit networks described by the XYZ Hamiltonian and we find a full characterization of the chains admitting pretty good state transfer, namely we prove the following result:

Theorem 1. *Pretty good state transfer occurs between the extremal vertices of Heisenberg chain of n qubits if and only if n is prime congruent to 1 modulo 4 or a power of 2. Moreover,*

in these cases, pretty good state transfer occurs between vertices at the j th and $(n + 1 - j)$ th position for all $j = 1, \dots, n$.

The remainder of the paper is organized as follows. In Section II we introduce the required notation. Section III describes the tools needed for the proof of our main result. Specifically Theorem 2 generalizes for every symmetric algebraic matrix a result by Vinet and Zhedanov⁸ on XY spin chains. Finally Section IV proves our main result.

II. NOTATION

We consider a graph $G = (V, E)$ with a set of vertices $V(G) = \{1, \dots, n\}$ and a set of edges $E(G)$ that describe the physical pairwise couplings between two vertices. We denote $A(G)$ the adjacency matrix with elements $[A(G)]_{ij} = 1$, if $(i, j) \in E(G)$, and $[A(G)]_{ij} = 0$ otherwise. For a generic graph structure the Heisenberg (XYZ) Hamiltonian is defined by

$$\mathcal{H}_{\text{XYZ}}(G) = \frac{1}{2} \sum_{i \neq j} A(G)_{ij} (X_i X_j + Y_i Y_j + Z_i Z_j), \quad (1)$$

where X_i, Y_i, Z_i are the Pauli matrices acting on the i -th vertex. On the other hand, the XY Hamiltonian is

$$\mathcal{H}_{\text{XY}}(G) = \frac{1}{2} \sum_{i \neq j} A(G)_{ij} (X_i X_j + Y_i Y_j). \quad (2)$$

Both $\mathcal{H}_{\text{XY}}(G)$ and $\mathcal{H}_{\text{XYZ}}(G)$ act on the Hilbert space $(\mathbb{C}^2)^{\otimes n}$. We call $\{|0\rangle, |1\rangle\}$ the basis of the Pauli matrices on each vertex and we define the single-particle subspace as the Hilbert space generated by the vectors $X_i|0\rangle^{\otimes n} = |0 \dots 010 \dots 0\rangle \in (\mathbb{C}^2)^{\otimes n}$, for $i = 1, \dots, n$, where the $|1\rangle$ state is in the i -th position. Within this single-particle subspace, the above Hamiltonians can be written as (see Ref.⁶)

$$\mathcal{H}_{\text{XYZ}}^{(1)}(G) = |E(G)|\mathbb{1} - 2L(G), \quad (3)$$

$$\mathcal{H}_{\text{XY}}^{(1)}(G) = 2A(G), \quad (4)$$

where the subscript (1) refers to the single-particle subspace, $L(G) = \Delta(G) - A(G)$ is the Laplacian of the graph and $\Delta(G)$ is the diagonal matrix whose diagonal i -th entry is the degree $d(i)$ of vertex i , namely the number of edges incident with i . For simplicity, we avoid the use of the explicit notation $\mathcal{H}_{\text{XYZ}}^{(1)}(G)$, $\mathcal{H}_{\text{XY}}^{(1)}(G)$, and we simply call $A(G)$ and $L(G)$ as

the XY and XYZ Hamiltonians, as they are equivalent to equations ((1)) and ((2)) in the single-particle subspace up to a trivial rescaling and shift.

We now introduce the concept of perfect and pretty good state transfer. Given M a symmetric matrix whose columns are indexed by the set of vertices V , we say that *perfect state transfer* occurs between vertices a and b of M if there is a $\tau \in \mathbb{R}^+$ such that

$$|\exp(i\tau M)_{a,b}| = 1.$$

This framework generalizes the concept of state transfer in the quantum walk of XY and XYZ Hamiltonians in the single-excitation subspace where M is respectively chosen as $A(G)$ or $L(G)$. If it is clear from the context which M we are dealing with, we use the notation $\exp(itM) = U(t)$.

We relax the definition of perfect state transfer to an ϵ -version. We say that M admits *pretty good state transfer* (also known as almost perfect state transfer) between vertices a and b if, for any $\epsilon > 0$, there is a time $\tau > 0$ such that

$$|U(\tau)_{a,b}| > 1 - \epsilon, \tag{5}$$

If \mathbf{e}_a and \mathbf{e}_b are the characteristic vectors of columns a and b , equation (5) is equivalent to the existence of a $\lambda \in \mathbb{C}$ of absolute value equal to 1 such that

$$\|U(\tau)\mathbf{e}_a - \lambda\mathbf{e}_b\| < \epsilon.$$

Finally, for shortness, when ϵ is not relevant, we abbreviate this equation to

$$U(\tau)\mathbf{e}_a \approx \lambda\mathbf{e}_b.$$

Godsil et al.⁹ determined when a linear chain with unmodulated spins admits pretty good state transfer between the end vertices according to the XY-Hamiltonian. Subsequently, Vinet and Zhedanov⁸ worked on chains with non-unitary weights, providing new examples of pretty good state transfer in the XY-Hamiltonian model.

In this paper, we review a known characterization of pretty good state transfer in detail, and as a result, we fully characterize linear chain with unmodulated spins admitting pretty good state transfer according to the Heisenberg Hamiltonian.

III. TECHNICAL PRELIMINARIES

Given a real symmetric matrix M , with spectral decomposition

$$M = \sum_{r=0}^d \theta_r E_r,$$

we say that a and b are *strongly cospectral* if $E_r \mathbf{e}_a = \pm E_r \mathbf{e}_b$ for all r . This nomenclature is inspired by the following fact. We say that vertices a and b are *cospectral* if the matrix obtained from M upon removing row and column indexed by a has the same spectrum as when we remove row and column indexed by b . An equivalent formulation is that $(E_r)_{a,a} = (E_r)_{b,b}$ for all r , therefore every pair of strongly cospectral vertices is cospectral, as one would expect. If M is either the adjacency or the Laplacian matrix of a graph, cospectral vertices have necessarily the same number of neighbours. Moreover, in the adjacency case, a and b are cospectral if and only if, for all $k \in \mathbb{Z}$, the number of walks of length k that start and end in a is the same as the number for b (see Ref.¹⁸ (Section 2.5) for proofs and references of these facts). There are cases in which cospectral vertices are not strongly cospectral, and in fact we do not know any combinatorial characterization of this property. Finally, it is worth mentioning that if all eigenvalues are simple, both properties are equivalent, and that if M is a tridiagonal matrix (thus encoding the adjacency of a linear chain), then strong cospectrality is equivalent to the property of mirror-symmetry of the weights.

We also define the *eigenvalue support* of a as the set of eigenvalues θ_r such that $E_r \mathbf{e}_a \neq 0$.

To prove our main result, we use the following characterization of pretty good state transfer. The core of the result is a theorem due to Kronecker. It has already been applied to study quantum walks. For instance, the restriction of this characterization to study pretty good state transfer in the adjacency matrix of XY chains with arbitrary weights was used by Vinet and Zhedanov⁸. Here we extend its usage to a very general case.

Theorem 2. *Let a and b be columns of a symmetric algebraic matrix M . Then pretty good state transfer occurs between a and b if and only if*

- (i) *Columns a and b are strongly cospectral. In this case, let $\theta_0, \dots, \theta_d$ be the eigenvalues in their support, and for $r = 0, \dots, d$, let σ_r be defined as 0 if the projections onto E_r are equal, and 1 if they have opposite signs.*

(ii) If there is a set of integers ℓ_0, \dots, ℓ_d such that

$$\sum_{r=0}^d \ell_r \theta_r = 0 \quad \text{and} \quad \sum_{r=0}^d \ell_r \sigma_r \text{ is odd,}$$

then

$$\sum_{r=0}^d \ell_r \neq 0,$$

and, if 2^α is the largest power of 2 dividing $\sum_{r=0}^d \ell_r$, then for any other set of integers j_0, \dots, j_d satisfying $\sum_{r=0}^d j_r \theta_r = 0$, if 2^β is the largest power of 2 dividing $\sum_{r=0}^d j_r$ (assuming $\beta = \infty$ if the sum is equal to 0), then $\beta \geq \alpha$, with equality if and only if $\sum_{r=0}^d j_r \sigma_r$ is odd.

We will see that for Heisenberg chains, condition (ii) can be significantly simplified. So bear with us. But before, we show that (i) is a necessary condition.

Lemma 3. *If pretty good state transfer occurs between a and b , then they are strongly cospectral vertices.*

Proof. From the spectral decomposition, we have

$$U(t) = \sum_{r=0}^d e^{it\theta_r} E_r,$$

thus

$$|U(t)_{a,b}| \leq \sum_{r=0}^d |(E_r)_{a,b}|.$$

Now $\sum E_r = I$, and, by Cauchy-Schwartz,

$$(E_r)_{a,a} \geq |(E_r)_{a,b}|.$$

Thus

$$\sum_{r=0}^d |(E_r)_{a,b}| = 1$$

if and only if, for all r ,

$$(E_r)_{a,a} = |(E_r)_{a,b}|,$$

or equivalently, a and b are strongly cospectral. As pretty good state transfer means that $|U(t)_{a,b}|$ gets arbitrarily close to 1 for some values of t , the result follows. \square

We make use of the following result due to Kronecker.

Theorem 4 (Kronecker, see for instance Ref.¹⁹, Chapter 3). *Let $\theta_0, \dots, \theta_d$ and ζ_0, \dots, ζ_d be arbitrary real numbers. For an arbitrarily small ϵ , the system of inequalities*

$$|\theta_r y - \zeta_r| < \epsilon \pmod{2\pi}, \quad (r = 0, \dots, d),$$

admits a solution for y if and only if, for integers ℓ_0, \dots, ℓ_d , if

$$\ell_0 \theta_0 + \dots + \ell_d \theta_d = 0,$$

then

$$\ell_0 \zeta_0 + \dots + \ell_d \zeta_d \equiv 0 \pmod{2\pi}.$$

Now we prove our characterization.

Proof of Theorem 2. Observe that

$$U(\tau) \mathbf{e}_a \approx \lambda \mathbf{e}_b$$

is equivalent to, for all r ,

$$e^{i\theta_r \tau} E_r \mathbf{e}_a \approx \lambda E_r \mathbf{e}_b,$$

which in turn, when $\lambda = e^{i\delta}$, is equivalent to, for all r such that $E_r \mathbf{e}_a \neq 0$,

$$\theta_r \tau \approx \delta + q_r \pi, \tag{6}$$

where $q_r \in \mathbb{Z}$ is even if and only if $E_r \mathbf{e}_a = E_r \mathbf{e}_b$, and odd if and only if $E_r \mathbf{e}_a = -E_r \mathbf{e}_b$.

A solution to equation (6) is equivalent to a solution as described in Theorem 4 with

$$y = \tau \quad \text{and} \quad \zeta_r = \delta + \sigma_r \pi,$$

where $\sigma_r = 0$ if $E_r \mathbf{e}_a = E_r \mathbf{e}_b$, and $\sigma_r = 1$ if $E_r \mathbf{e}_a = -E_r \mathbf{e}_b$.

Now, a set of integers ℓ_0, \dots, ℓ_d satisfies

$$\ell_0 \zeta_0 + \dots + \ell_d \zeta_d \equiv 0 \pmod{2\pi}$$

if and only if there is a δ such that

$$\ell_0(\delta + \sigma_0 \pi) + \dots + \ell_d(\delta + \sigma_d \pi) \equiv 0 \pmod{2\pi}$$

which in turn is equivalent to

$$\delta \left(\sum_{r=0}^d \ell_r \right) + \pi \left(\sum_{r=0}^d \sigma_r \ell_r \right) \equiv 0 \pmod{2\pi}. \quad (7)$$

A choice of δ that solves equation (7) for all sets of integers ℓ_0, \dots, ℓ_d satisfying $\sum \ell_r \theta_r = 0$ is possible if and only if, whenever $\sum_{r=0}^d \sigma_r \ell_r$ is odd, $\delta \sum_{r=0}^d \ell_r$ is an odd multiple of π , and whenever $\sum_{r=0}^d \sigma_r \ell_r$ is even, $\delta \sum_{r=0}^d \ell_r$ is an even multiple of π . This proves that if (i) holds, then (ii) is equivalent to pretty good state transfer. \square

This next corollary is notably useful to study the Laplacian matrix.

Corollary 5. *Assume that 0 is an eigenvalue of M in the support of strongly cospectral columns a and b . Say the other eigenvalues in their support are $\theta_1, \dots, \theta_d$, and have $\sigma_1, \dots, \sigma_d$ defined as before. Then pretty good state transfer occurs between a and b if and only if whenever there are integers ℓ_1, \dots, ℓ_d such that*

$$\sum_{r=1}^d \ell_r \theta_r = 0,$$

then

$$\sum_{r=1}^d \sigma_r \ell_r \text{ is even.}$$

Moreover, in this case, the complex phase with which pretty good state transfer occurs will be equal to 1.

Proof. Make $\theta_0 = 0$. Then given ℓ_0, \dots, ℓ_d ,

$$\sum_{r=0}^d \ell_r \theta_r = 0 \iff \sum_{r=1}^d \ell_r \theta_r = 0.$$

Hence the choice of ℓ_0 is arbitrary, and thus can always be made such that

$$\sum_{r=0}^d \ell_r = 0.$$

Thus, in order for pretty good state transfer to occur, $\sum_{r=1}^d \sigma_r \ell_r$ can never be odd, and if it is even in all cases, condition (ii) of Theorem 2 is vacuously satisfied. Moreover, in this case, as the choice ℓ_0 is arbitrary and hence can also be made in a way that $\sum_{r=0}^d \ell_r$ is odd, δ must be an even multiple of π , therefore $\lambda = e^{i\delta} = 1$. \square

A. The spectrum of Heisenberg chains

We refer the reader to Brouwer and Haemers²⁰ for the result below. Let P_n denote the path on n vertices. Recall that $L(X)$ denotes the Laplacian matrix of the graph X .

- The eigenvalues of $L(P_n)$ are 0 with the all 1s eigenvector, and $2 + 2\cos(\pi r/n)$, $r = 1, \dots, n-1$. If $\beta_k = \sin(k\pi r/n)$, its corresponding eigenvector is

$$(\beta_1, (-1)^1(\beta_1 + \beta_2), (\beta_2 + \beta_3), \dots, (-1)^n(\beta_{n-2} + \beta_{n-1}), (-1)^{n+1}\beta_{n-1}).$$

IV. MAIN RESULT

We are ready to prove Theorem 1.

Theorem 1 (restated) *Pretty good state transfer occurs on $L(P_n)$ between the extremal vertices if and only if n is prime congruent to 1 modulo 4 or a power of 2. Moreover, in these cases, pretty good state transfer occurs between vertices at the j th and $(n+1-j)$ th position for all $j = 1, \dots, n$.*

Proof. Suppose the spectral decomposition of $L(P_n)$ is given by

$$L(P_n) = \sum_{r=0}^{n-1} \lambda_r E_r.$$

Let R be the anti-diagonal matrix of order n . It is a straightforward consequence of the spectrum of P_n described in Section III A that

$$\sum_{r=0}^{n-1} (-1)^r E_r = R.$$

This readily implies that vertices at positions j and $(n+1-j)$ are strongly cospectral for $j = 1, \dots, n$, and hence condition (i) of Theorem 2 is always satisfied, with $\sigma_r = (-1)^r$.

Let $\zeta_{2n} = e^{\pi/n}$. Clearly the eigenvalues of P_n can be expressed as

$$\lambda_r = 2 - (\zeta_{2n}^r + \overline{\zeta_{2n}^r}) = 2 - (\zeta_{2n}^r + \zeta_{2n}^{2n-r}).$$

As a consequence, the eigenvalues belong to the cyclotomic field of ζ_{2n} . Now assume there are integers $\ell_1, \dots, \ell_{n-1}$ such that

$$\sum_{r=1}^{n-1} \ell_r (-2 + (\zeta_{2n}^r + \zeta_{2n}^{2n-r})) = 0. \quad (8)$$

If $\ell_0 = -\sum_{r=1}^{n-1} \ell_r$, then the cyclotomic polynomial $\Phi_{2n}(x)$ divides

$$L(x) = 2\ell_0 + \sum_{r=1}^{n-1} \ell_r x^r + \sum_{r=n+1}^{2n-1} \ell_{2n-r} x^r. \quad (9)$$

- If n is a power of 2, then $\Phi_{2n}(x) = 1 + x^n$. Performing long division starting from the terms of smaller degree, the general form of an exact quotient of the division of $L(x)$ by $\Phi_{2n}(x)$ is

$$2\ell_0 + \sum_{r=1}^{n-1} \ell_r x^r,$$

thus the division is exact (and equation (8) is satisfied) if and only if $\ell_0 = 0$ and $\ell_s = \ell_{n-s}$ for all $s = 1, \dots, n$. As a consequence, whenever (8) holds, $\sum \ell_{\text{odd}}$ is always even, and pretty good state transfer occurs.

- If n is an odd prime, then $\Phi_{2n}(x) = 1 - x + x^2 - \dots + x^{n-1}$. Performing long division starting from the terms of smaller degree, the general form of an exact quotient of the division of $L(x)$ by $\Phi_{2n}(x)$ is

$$2\ell_0 + (2\ell_0 + \ell_1)x + \sum_{r=2}^{n-1} (\ell_r + \ell_{r-1})x^r + \ell_1 x^n.$$

This implies that a set of integers $\ell_1, \dots, \ell_{n-1}$ satisfy equation (8) if and only if, for all odd s between 1 and $n-1$,

$$\ell_s - \ell_{n-s} = -2\ell_0 = 2 \sum_{r=1}^{n-1} \ell_r. \quad (10)$$

If $n \equiv 3 \pmod{4}$, then $\ell_{\text{odd}} = n$ and $\ell_{\text{even}} = -(n-2)$ provides a solution such that

$$\sum \ell_{\text{odd}} \text{ is odd,}$$

hence pretty good state transfer does not occur in this case.

If $n \equiv 1 \pmod{4}$, the analysis is more delicate. Let $A = \sum \ell_{\text{odd}}$ and $B = \sum \ell_{\text{even}}$. From equation (10) it follows that

$$A - B = (n-1)(A + B).$$

Suppose A is odd. Because $(n-1) \equiv 0 \pmod{4}$, it follows that $A \equiv B \pmod{8}$. Hence $2(A+B) \equiv 4 \pmod{8}$. With s odd, equation (10) and the fact that A is odd imply

that there is an odd number of pairs (ℓ_s, ℓ_{n-s}) such that either $\ell_s \equiv \ell_{n-s} \equiv 1 \pmod{4}$ or $\ell_s \equiv \ell_{n-s} \equiv 3 \pmod{4}$, but not both. Say the former (the latter is analogous). Suppose there are M pairs with $\ell_s \equiv 1 \pmod{8}$ and $\ell_{n-s} \equiv 5 \pmod{8}$, and N pairs with $\ell_s \equiv 5 \pmod{8}$ and $\ell_{n-s} \equiv 1 \pmod{8}$. As $M + N$ is odd, suppose without loss of generality that $M > N$, and thus $M - N$ is odd. Hence there is an even number P such that

$$A \equiv (M - N) + P \pmod{8} \quad \text{and} \quad B \equiv 5(M - N) + P \pmod{8}.$$

A contradiction to the fact that $A - B \equiv 0 \pmod{8}$. Therefore A must be even, and pretty good state transfer occurs in this case.

- Now suppose $n = mj$, with m odd, $m > 1$ and $j > 1$. Let p be an odd prime dividing m , thus $2n = pk$, with k a positive even number. It follows that $x^{2n} - 1 = \Phi_p(x)R(x)$ where

$$R(x) = \sum_{t=0}^{k-1} -x^{tp} + x^{tp+1}.$$

Let ℓ_r be defined as 0, 1 or -1 in such way that

$$R(x) = \sum_{r=0}^{n-1} \ell_r x^r.$$

Note that 1, ζ_{2n} and ζ_{2n}^{2n-1} are all roots of $R(x)$. Thus

$$R(\zeta_{2n}) + R(\zeta_{2n}^{2n-1}) = 0 \quad \text{and} \quad \sum_{r=1}^{n-1} \ell_r = 1.$$

Hence

$$0 = R(\zeta_{2n}) + R(\zeta_{2n}^{2n-1}) = \sum_{r=1}^{n-1} \ell_r (-2 + \zeta_{2n}^r + \zeta_{2n}^{2n-r})$$

where, for $t = 1, \dots, k - 1$,

$$\ell_r = 1 \text{ if } r = tp + 1, \quad \ell_r = -1 \text{ if } r = tp, \quad \ell_r = 0 \text{ otherwise.}$$

Note that t is odd if and only if tp is odd, and t is even if and only if $tp + 1$ is odd. Thus the sum of the ℓ_r with odd r is equal to -1 . Therefore pretty good state transfer does not occur in this case.

□

We point out that we are not necessarily determining all cases in which a qubit chain might admit pretty good state transfer, as we are focusing only on transfer between the end vertices. In fact, it seems that the problem of characterizing pretty good state transfer between inner vertices was not solved for the XY-Hamiltonian either. We leave this as an open question.

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