Exact solution of a family of staggered Heisenberg chains with conclusive pretty good quantum state transfer

Pablo Serra(1), Alejandro Ferrón(2), and Omar Osenda(1)

(1) Instituto de Física Enrique Gaviola (CONICET-UNC) and Facultad de Matemática, Astronomía, Física y Computación, Universidad Nacional de Córdoba, Av. Medina Allende s/n, Ciudad Universitaria, CP:X5000HUA Córdoba, Argentina

(2) Instituto de Modelado e Innovación Tecnológica (CONICET-UNNE) and Facultad de Ciencias Exactas, Naturales y Agrimensura, Universidad Nacional del Nordeste, Avenida Libertad 5480, W3404AAS Corrientes, Argentina.

(Dated: June 30, 2022)

We construct the exact solution for a family of one-half spin chains explicitly. The spin chains Hamiltonian corresponds to an isotropic Heisenberg Hamiltonian, with staggered exchange couplings that take only two different values. We work out the exact solutions in the one-excitation subspace. Regarding the problem of quantum state transfer, we use the solution and some theorems concerning the approximation of irrational numbers, to show the appearance of conclusive pretty good transmission for chains with particular lengths. We present numerical evidence that pretty good transmission is achieved by chains whose length is not a power of two. The set of spin chains that shows pretty good transmission is a subset of the family with an exact solution. Using perturbation theory, we thoroughly analyze the case when one of the exchange coupling strengths is orders of magnitude larger than the other. This strong coupling limit allows us to study, in a simple way, the appearance of pretty good transmission. The use of analytical closed expressions for the eigenvalues, eigenvectors, and transmission probabilities allows us to obtain the precise asymptotic behavior of the time where the pretty good transmission is observed. Moreover, we show that this time scales as a power law whose exponent is an increasing function of the chain length. We also discuss the crossover behavior obtained for the pretty good transmission time between the regimes of strong coupling limit and the one observed when the exchange couplings are of the same order of magnitude.

PACS numbers:

I. INTRODUCTION

The Heisenberg model has been studied in the context of the Quantum state Transfer in a host of works [1–3], with different strategies that go from rigorous results and theorems [4–7] to completely numerical efforts. Even the availability of the Bethe ansatz, and the integrability of the model, can not hide the fact that the autonomous evolution of homogeneous Heisenberg chains is ill-suited to perform Quantum State Transfer (QST) with very high fidelity and short transfer times. The XX chains, on the contrary, allow perfect quantum state transfer using different strategies [8–11] or near perfect QST at transfer times close to the minimal time allowed by the Quantum Speed limit [12–14]. Regrettably, more and more experimental implementations can be modeled only by using effective Heisenberg chain Hamiltonians [15–25] (or more complicated interactions [26–28]) while the XX chains remain as an option only for simplistic highly anisotropic situations. Of course, there is always room for renewed proposals that involve the XX Hamiltonian, as is the case in some XX chains that show topological states [26–28].

On the other hand, much progress have been made concerning the non-autonomous time evolution of spin chains [29–31], although many times the control leads to particular results about the times for which the transfer is achievable [29–33]. The controllability of the dynamics is a well studied area with numerous results [29–37].

The basic difficulty of the homogeneous Heisenberg chains mentioned above has driven the study of some alternatives and the formulation of a specialized jargon that classifies the different dynamical scenarios that arise when non-homogeneous chains are considered or the condition of a short (and known) arrival time is lifted [4–7]. The pretty good QST [4–6] and fractional revival [38, 39] are two of the most studied scenarios, the spectral conditions needed to their appearance are well understood. Nevertheless, these conditions do not prescribe, for instance, how the different exchange coefficients must be selected to achieve the pretty good scenario nor the precise arrival time at which the QST is effectively observed or how this time could scale with the two main parameters of the chain, the largest interaction strength, and its length.

Heisenberg spin chains with nearest-neighbor time-independent staggered, or alternating, exchange coefficients are easier to implement than chains with all their spin coupling interactions tuned to precise values, at least in principle. Despite that the tailoring of all couplings can be, in principle, achieved in some implementations and result in near-perfect QST at known times [40–41], in this paper we aim to study the simpler staggered case, when the exchange...
couplings can take only two alternating values, $J_1$ and $J_2$. The typical chain has an exchange coupling (EC) equal to $J_1$ between the first and second spin, $J_2$ between the second and third spin, and so on. The sequence described results in a centrosymmetric chain if the number of spins is even, with the central EC equal to $J_2$.

First, we will show that for particular families of chain lengths the spectrum and eigenvalues of the problem restricted to a subspace of the whole Hilbert space can be calculated exactly using rather simple means. More importantly, the functional dependency of the eigenvalues with the parameters allows for a detailed analysis of the properties of the QST process through the population transfer. Using theorems about the best rational approximation that can be achieved for irrational numbers we can explicitly show the appearance of the pretty good QST scenario for small chains. Besides we can calculate explicitly the arrival time, i.e. we obtain the time $t_\star$ such that the population transferred satisfies $P(t_\star) < 1 - \epsilon$. Interestingly, for small chains, it is possible to show that the scenario appears for almost any value of the parameter $J_2$ while keeping $J_1 = 1$ and for chains with $N = 2^k$ and $N = \alpha \times 2^k$, with $\alpha = 3$ or 5. This last result shows that the family of spin chains possessing PGT is larger than previously reported.

Later, we present analytical results for the population transferred in the limit $J_2 \rightarrow \infty$. We call this regime the strong coupling limit. We work out the results using perturbation theory and show that the population transferred in the strong coupling limit has a simpler structure and dependency with the eigenvalues than the exact results. The strong coupling limit allows us to study chains of arbitrary length. We present evidence that the population in the strong coupling limit also shows pretty good QST. Together with the results found for small chains, we conjecture the scaling of $t_\star \sim 1/(\epsilon)^{f(N)}$, where $f(N)$ is a simple function of the chain length.

II. THE QUANTUM STATE TRANSFER PROTOCOL AND THE TRANSFERRED POPULATION

We focus our study on the well-known Heisenberg quantum spin chain Hamiltonian,

$$H = -\sum_{i=1}^{N-1} J_i \vec{\sigma}_i \cdot \vec{\sigma}_{i+1}$$

(1)

where $J_i > 0$. The spectral and transfer properties of this Hamiltonian have been extensively studied, in particular when the chains are homogeneous, i.e. all the $J_i$ coefficients in Eq. (1) are equal ($J_i = J, \forall i$). The homogeneous chain is quite poor as a transfer channel when the simplest transfer protocol is used.

The Hamiltonian in Eq. (1) commute with the total magnetization in the $z$-direction

$$\left[ H, \sum_i \sigma_i^z \right] = 0,$$

(2)

so it can be diagonalized in subspace with fixed number of excitations, i.e. in subspaces with a given number of spins up. It is customary to use the computational basis, where for a single spin $|0\rangle = | \downarrow \rangle$ and $|1\rangle = | \uparrow \rangle$, so $|0\rangle = |0000\ldots0\rangle$ is the state with zero spins up of the whole chain.

Throughout this paper, we will work in the single excitation Hilbert space and study $h$, the $N \times N$ matrix of this block. We are mainly interested in finding the exact eigenvalues and eigenvectors of $h$ and using them to study transmission in this kind of spin chain. We understand that an exactly-solvable spin chain is one such that its eigenvalues and eigenvectors have an analytic expression. Once we have the eigenvalues and eigenvectors we should analyze the transmission properties of our spin chain. So we introduce a quantity that describes the transmission probability between an initial state and a final state. The $N$ states with a single spin up are denoted as follows

$$|1\rangle = |10\ldots0\rangle, |2\rangle = |010\ldots0\rangle, \ldots, |N\rangle = |00\ldots1\rangle.$$  

(3)

i.e. the state $|j\rangle$ is the state of the chain with only the $j$-th spin up. In the protocol studied along this paper the initial state of the chain, $|\Psi(0)\rangle$, is prepared as

$$|\Psi(0)\rangle = |\psi(0)\rangle \otimes |0\rangle_{N-1},$$

(4)

where $|\psi(0)\rangle = |1\rangle$ is an excitation in the first site of the chain and $|0\rangle_{N-1}$ is the state without excitations of a chain with $N - 1$ spins. The state in Eq. (1) can be rewritten as
\[ |\Psi(0)\rangle = |1\rangle. \] (5)

Using the time evolution operator
\[ U(t) = \exp(-iHt), \] (6)
the state of the chain at time \( t \) can be obtained as
\[ |\Psi(t)\rangle = U(t)|\Psi(0)\rangle = U(t)|1\rangle. \] (7)
and we define the transferred population (TP) between the first and last sites of the chain as
\[ P(t) = |\langle 1 | U(t) | N \rangle|^2, \] (8)
this is our quantity of interest. Perfect transmission (PT) is achieved when \( P(t) = 1 \) for some time. The scenario known as pretty good quantum state transfer (PGT) occurs if for some time \( t_\epsilon \)
\[ P(t_\epsilon) = 1 - \epsilon, \quad \forall \epsilon > 0. \] (9)

III. EXACT SOLUTION FOR SPIN CHAINS WITH STAGGERED EXCHANGE COUPLING COEFFICIENTS

In this paper, we focus on non-homogeneous spin chains obtaining analytical and closed expressions for eigenvalues, eigenvectors, and transferred population or transmission probabilities. It is important to note that it is always possible to take \( J_k = 1 \) for some \( k \), so chains with \( N = 2 \) have no free parameters, and chains with \( N = 3 \) have just one free parameter (\( J_1 = 1; J_2 \) free). It is easy to show that, for \( N = 4 \), there is no analytically closed solution when \( J_1 = 1 \) and \( J_2, J_3 \) are arbitrary parameters. Obtaining analytical expressions in a completely general scenario would be impossible. We start asking for centrosymmetric spin chains as in most of our previous works [34, 40, 41]

\[ J_{N-i} = J_i; \quad i = 1, \ldots, [N/2]. \] (10)
With this convention, the matrix \( h \) results bisymmetric, and the spin chains with \( N = 4, 5 \) are now exactly-solvable. Anyway, \( N \geq 6 \) has no analytical expressions for its eigenvalues and eigenvectors. We will show that the bisymmetric spin chains are exactly-solvable when their length is \( N = \alpha \times 2^k \), with \( \alpha \) and \( k \) natural numbers. We choose centrosymmetric chains with
\[ J_{2i-1} = 1 \quad J_{2i} = J_2; \quad i = 1, \ldots, N/2; \quad N \in 2\mathbb{N}. \] (11)
In this case, the corresponding matrix \( h^{(N)} \) can be written as:
\[
\begin{pmatrix}
0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 \\
-2 & d^{(N)} + 2J_2 & -2J_2 & 0 & 0 & \ldots & 0 & 0 \\
0 & -2J_2 & d^{(N)} + 2J_2 & -2 & 0 & \ldots & 0 & 0 \\
0 & 0 & -2 & d^{(N)} + 2J_2 & -2J_2 & 0 & \ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \ldots & 0 & d^{(N)} + 2J_2 & -2J_2 \\
0 & 0 & 0 & 0 & \ldots & -2J_2 & d^{(N)} + 2J_2 & -2 \\
0 & 0 & 0 & 0 & \ldots & 0 & -2 & d^{(N)} \\
\end{pmatrix},
\] (12)
where
\[ d^{(N)} = - \left( \frac{N}{2} - 2 \right) - \left( \frac{N}{2} - 1 \right) J_2. \]  

It is convenient to define the matrix

\[
\mathbf{h}^{(N)} = \mathbf{h}^{(N)} - (d^{(N)} + 2 J_2) \mathbb{I}_N,
\]

because its elements do not depend on \( N \). Clearly, if \( \lambda \) is an eigenvalue of \( \mathbf{h}^{(N)} \), then \( \lambda + d^{(N)} + 2 J_2 \) is an eigenvalue of \( \mathbf{h}^{(N)} \), and both matrices have the same eigenvectors. \( \mathbf{h}^{(N)} \), and then \( \mathbf{h}^{(N)} \), are bisymmetric matrices, then we can write:

\[
\mathbf{h}^{(N)} = \begin{pmatrix} A & B \\ B^t & S A S \end{pmatrix},
\]

where the \( N/2 \times N/2 \) matrices \( A, B \) and \( S \) are

\[
A = \begin{pmatrix} -2 J_2 & -2 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ -2 & 0 & -2 J_2 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -2 J_2 & 0 & -2 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & -2 J_2 & 0 & -2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & b & 0 & a \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & a & 0 \end{pmatrix},
\]

\[
B = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ b & 0 & 0 & \cdots & 0 \end{pmatrix}; \quad S = \begin{pmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 0 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 \end{pmatrix},
\]

where \( a \) and \( b \) are constants depending on the parity of \( N/2 \),

\[
a = \begin{cases} -2 & \text{if } N/2 \text{ is even} \\ -2 J_2 & \text{if } N/2 \text{ is odd} \end{cases}; \quad b = \begin{cases} -2 J_2 & \text{if } N/2 \text{ is even} \\ -2 & \text{if } N/2 \text{ is odd} \end{cases}.
\]

Now, defining \( A_{\pm}^{(N/2)} = A \pm B S \) we know that the eigenvalues of \( A_{-}^{(N/2)} \) and \( A_{+}^{(N/2)} \) are the eigenvalues of \( \mathbf{h}^{(N)} \) \[^{42}\].

In the particular case where \( N/2 \) is even, we have the important relation

\[
A_{+}^{(N/2)} = \mathbf{h}^{(N/2)},
\]

that is, if we know the eigenvalues of \( \mathbf{h}^{(N/2)} \), to know the eigenvalues of \( \mathbf{h}^{(N)} \) we only need to calculate the eigenvalues of \( A_{-}^{(N/2)} \). By inspection, we corroborate that, for even values of \( N \), the eigenvalues of \( \mathbf{h}^{(N)} \) can be written as

\[
\lambda_{-}^{(m)} = -2 \sqrt{1 + J_2^2 + 2 J_2 \cos \left( \frac{2 m \pi}{N} \right)}; \quad m = 0, \ldots, \frac{N}{2}
\]

\[
\lambda_{+}^{(m)} = 2 \sqrt{1 + J_2^2 + 2 J_2 \cos \left( \frac{2 m \pi}{N} \right)}; \quad m = 1, \ldots, \frac{N}{2} - 1.
\]
For the case $N/2$ even, the eigenvalues of $A_{(N/2)}$ are given by the odd values of $m$,

$$\lambda^{(2l+1)}_{\pm} = \pm 2 \sqrt{1 + J_2^2 + 2 J_2 \cos \left( \frac{(2l + 1) \pi}{N/2} \right)} : l = 0, \ldots, \frac{N}{4} - 1.$$  \hspace{1cm} (21)

We keep the notation $E_m; m = 1, \ldots, N$, for the eigenvalues of $h$, with this convention they will be ordered from smallest to greatest.

From now on, we will pay particular attention to chains with $N/2$ an even number. As we will see below, we can state that, for

$$N = 2n = \alpha 2^k ; \ k \in \mathbb{N},$$

and $\alpha$ takes one of the values

$$\alpha = \left\{ \frac{2}{3^p \times 5^q \times 17^r \times 257^s \times 65537^t} ; \ p, q, r, s, t = 0, 1 \right\},$$

(23)

The list of elements of $\alpha$ values smaller than 1000 reads as follows

$$\alpha = 2, 3, 5, 15, 17, 51, 85, 255, 257, 771.$$ \hspace{1cm} (24)

We want to remark here that, for these values of $\alpha$, there is an algebraic expression for the cosine functions in Eq. (20) (see Appendix A). This allow us to write down algebraic expressions for all the eigenvalues and eigenvectors coefficients on which the TP depends.

The following section deals with some particular cases of $\alpha$. We will pay close attention to the smallest values of this list, $\alpha = 2, 3$ and 5, as a showcase of the methods employed to analyze chains of moderate length ($N \simeq 20, 30$). These methods rely on the Dirichlet’s Approximation Theorem for irrational numbers and the algebraic representation of particular values of trigonometric functions.

**IV. EIGENVALUES, EIGENVECTORS AND TRANSMISSION PROBABILITIES**

In the previous section, we found analytical and simple expressions for the matrices corresponding to centrosymmetric Heisenberg spin chains such that $J_{2i-1} = 1$ and $J_{2i} = J_2$ for $i = 1, \ldots, N/2; \ N \in 2\mathbb{N}$. We also showed that these spin chains, with $N = \alpha 2^k; \ k \in \mathbb{N}$ and $\alpha$ taking values as in Eq. (23), are exactly solvable. It is worth noting that, by exactly-solvable, we mean that both eigenvalues and the eigenvectors have algebraic expressions. The consequences of having algebraic expressions for the eigenvalues will be clear once we introduce Dirichlet’s Approximation Theorem. We will dedicate this section to showing the explicit form of eigenvalues and eigenvectors of some of these spin chain Hamiltonians, and we will use them to analyze the transmission probability by constructing analytical expressions for $P(t)$ defined in Eq. (8). In the following we will use transferred population and transmission probability as equivalent terms. We can not take a look at all the possible spin chains, and because of that, we will pay particular attention to small values of $\alpha$ ($\alpha = 2, 3$ and 5) and some values of $k$.

**A. Chains with $N = 2 \times 2^k$ ($\alpha = 2, n = 2^k$)**

We will start with this relevant case, because it is known that it presents PGT for $J_2 = 1$ [6]. If we know the eigenvalues of $h^{(N/2)}$, then, using Eq. (19), we only need to calculate $N/2 = n$ new eigenvalues given by Eq. (21),

$$\lambda^{(m)}_{\pm} = \left\{ \pm 2 \sqrt{1 + J_2^2 + 2 J_2 \cos \left( \frac{(2m + 1) \pi}{2n} \right)} ; \ m = 0, \ldots, 2^{k-1} - 1 \right\},$$

(25)

or, equivalently, using the algebraic expression of the cosine functions (see Appendix A),
$$\{\lambda_{\pm}\}_1^{k-1} = \left\{ \pm 2 \sqrt{1 + J_2^2 + J_2 \sqrt{2 \pm \sqrt{2 \pm \ldots \pm \sqrt{2}}} \right\}, \quad (26)$$

with $N = 4$ as "initial condition", where all the eigenvalues are calculated explicitly. For this case, the Heisenberg Hamiltonian is given by

$$H = - (\vec{\sigma}_1 \cdot \vec{\sigma}_2 + J_2 \sigma_2^z \cdot \sigma_3^z + \sigma_3^z \cdot \sigma_4^z). \quad (27)$$

and we can write our Hamiltonian in the one excitation subspace as follow:

$$h^{(4)} = \begin{pmatrix} -J_2 & -2 & 0 & 0 \\ -2 & J_2 & -2J_2 & 0 \\ 0 & -2J_2 & J_2 & -2 \\ 0 & 0 & -2 & -J_2 \end{pmatrix} \Rightarrow h^{(4)} = \begin{pmatrix} -2J_2 & -2 & 0 & 0 \\ -2 & 0 & -2J_2 & 0 \\ 0 & -2J_2 & 0 & -2 \\ 0 & 0 & -2 & -2J_2 \end{pmatrix}. \quad (28)$$

The eigenvalues of $h^{(4)}$ are

$$\lambda^{(0)} = -2 - 2j2; \quad \lambda^{(1)} = -2 \sqrt{1 + J_2^2}; \quad \lambda^{(2)} = -2 + 2j2; \quad \lambda^{(1)} = 2 \sqrt{1 + J_2^2}. \quad (29)$$

Eigenvalues and eigenvectors of $h^{(4)}$, with the eigenvalues ordered from smallest one to largest one are:

$$E_1 = -2 - J_2; \quad |E_1\rangle = \frac{1}{2}(1, 1, 1, 1), \quad (30a)$$

$$E_2 = J_2 - 2\sqrt{1 + J_2^2}; \quad |E_2\rangle = C_2 \left(-1, J_2 - \sqrt{1 + J_2^2}, -J_2 + \sqrt{1 + J_2^2}, 1\right) \quad (30b)$$

$$E_3 = 2 - J_2; \quad |E_3\rangle = \frac{1}{2}(1, -1, -1, 1), \quad (30c)$$

$$E_4 = J_2 + 2\sqrt{1 + J_2^2}; \quad |E_4\rangle = C_4 \left(-1, J_2 + \sqrt{1 + J_2^2}, -(J_2 + \sqrt{1 + J_2^2}), 1\right) \quad (30d)$$

where

$$C_4 = \frac{1}{2\sqrt{1 + J_2^2 \pm J_2 \sqrt{1 + J_2^2}}} \quad (30e)$$

We can express the site basis as a linear combination of the eigenstates of the system. Then $|1\rangle$ and $|4\rangle$ should read as:

$$|1\rangle = \frac{1}{2} |E_1\rangle - C_2 |E_2\rangle + \frac{1}{2} |E_3\rangle - C_4 |E_4\rangle \quad (31)$$

$$|4\rangle = \frac{1}{2} |E_1\rangle + C_2 |E_2\rangle + \frac{1}{2} |E_3\rangle + C_4 |E_4\rangle.$$
Finally, using these expressions and, with the help of Equations (30), we can calculate $P(t) = |\langle 1|U(t)|4\rangle|^2$

$$P(J_2; t) = \frac{1}{8} \left\{ \cos \left[ 4t \right] + \frac{2 + 3J_2^2}{1 + J_2^2} \cos \left[ 4\sqrt{1 + J_2^2} t \right] - \frac{\cos \left[ 2(1 + J_2 - \sqrt{1 + J_2^2}) t \right] + \cos \left[ 2(1 - J_2 + \sqrt{1 + J_2^2}) t \right]}{1 + J_2^2 - J_2 \sqrt{1 + J_2^2}} \right. $$

$$\left. - \frac{\cos \left[ 2(1 + J_2 + \sqrt{1 + J_2^2}) t \right] + \cos \left[ 2(1 - J_2 - \sqrt{1 + J_2^2}) t \right]}{1 + J_2^2 + J_2 \sqrt{1 + J_2^2}} \right\} . \quad (32)$$

The PGT condition is satisfied if always exists a time $t_\varepsilon$, such that the value of the two cosine functions preceded by a plus sign are as close to the unity (the value of the four cosine functions preceded by a minus sign is as close to minus one) as required to obtain $P(t_\varepsilon) > 1 - \varepsilon$. Banchi and collaborators [6] proved that the case $J_2 = 1$ has PGT. However, they did not give any estimation for $t_\varepsilon$ and, for this reason, we include in our study the homogeneous chain.

In particular, to obtain PGT it is necessary that

$$\cos(4t_\varepsilon) \simeq 1 \Rightarrow t_\varepsilon \simeq \frac{m}{2} \pi \Rightarrow 2 \sqrt{1 + J_2^2} m \simeq l \ ; \ \left( 1 \pm J_2 \pm \sqrt{1 + J_2^2} \right) m \simeq 2l_{\pm\pm} + 1. \quad (33)$$

where $l$ and $l_{\pm\pm}$, and $m$ are natural numbers.

Dirichlet’s Approximation Theorem ensures the fulfillment of these conditions. The theorem says that

**Theorem 1** (Dirichlet’s Approximation Theorem) If $x_1, \ldots, x_m \in \mathbb{R}$ and $M \geq 1$ is an integer, then there exists an integer $q$ with $1 \leq q \leq M^m$ and integers $p_1, \ldots, p_m$ such that $|q x_i - p_i| < 1/M$ ; $i = 1, \ldots, m$.

The significance of this Theorem for our work is paramount. It assures us that some natural numbers fulfill the conditions in Eq. (33) and that the PGT time is $t_\varepsilon = q\pi$. Moreover, it is clear that the approximation of the irrational numbers is better for larger values of $M$. In other words, the larger the numbers $p_i$ and $q$ are considered, the better approximation results for the irrational numbers and the transmission probability.

The results about the PGT time included later in this work depend on the finding of successive approximations for the irrational numbers involved in the analytical expression of the transmission probabilities.

As shown in Appendix [A] (by Niven’s Theorem[13]) all the eigenvalues on which the transmission probabilities depend are functions of irrational numbers, see Eqs. (20) and (21). This dependency and the Dirichlet theorem give a systematic way to study chains with different lengths and values of the parameter $J_2$.

In what follows, we will continue dealing with the spin chain with only four spins, clarifying the use of the Theorem.

Note that, accordingly with (33) for $J_2$ equal to a natural number, the arguments of the cosine functions contain only a single irrational number $\sqrt{1 + J_2^2} = \sqrt{2}, \sqrt{5}, \sqrt{26}, \ldots$ for $J_2 = 1, 2, 5, \ldots$, respectively. In this simple case, the theorem assures that there are natural numbers $p$ and $q$ such that $|q\sqrt{1 + J_2^2} - p| < 1/M$.

For $J_2 = 1$, the condition that the second cosine function has a value close to the unity implies that

$$4\sqrt{2}t_\varepsilon = r\pi,$$

with $r$ an even number then, if $t_\varepsilon \simeq q\pi/2$ (that is, the condition that makes that the first cosine function has a value close to the unity) the second cosine function argument can be rewritten as

$$4\sqrt{2} \frac{\pi}{2} \simeq 2p\pi,$$

which leads to

$$\sqrt{2}q \simeq p.$$

The Theorem guarantees that this last equation is effectively fulfilled. It is rather direct to show that the conditions imposed by the other cosine functions that can be found in (33) are also fulfilled once a pair $(p, q)$ is found. So, it is clear that for a given pair of values $(p, q)$ such that $|q\sqrt{2} - p| < 1/M$ the time $t_\varepsilon = q\pi/2$ is a natural candidate to observe PGT. The actual value of $\varepsilon$ is calculated using that $\varepsilon = 1 - P(t_\varepsilon)$. 


There is a small number of algorithms to actually obtain the \((p, q)\) pairs. Fortunately, the best known is the one that allows to find rational approximations for \(\sqrt{2}\). The best rational approximations for \(\sqrt{2}\) are given by the Newton-Rapshon succession,

\[
a_0 = 1 \quad ; \quad a_{j+1} = \frac{a_j}{2} + \frac{1}{a_j} \quad ; \quad a_j = \frac{p_j}{q_j} \Rightarrow p_j = Num(a_j) ; q_j = Den(a_j),
\]

the first seven values of \(p_j, q_j\) are shown in Table I.

| \(j\) | \(p_j\) | \(q_j\) | \(|q_j - \sqrt{2}p_j|\) |
|-------|--------|--------|------------------|
| 0     | 1      | 1      | 0.41421          |
| 1     | 3      | 2      | 0.17157          |
| 2     | 17     | 12     | 0.02944          |
| 3     | 577    | 408    | 8.7 \times 10^{-4} |
| 4     | 665857 | 470832 | 7.5 \times 10^{-7} |
| 5     | 886731088897 | 627013566048 | |
| 6     | 1572584048032918633353217 | 1111984844349868137938112 | |

TABLE I: The successive approximations to \(\sqrt{2}\) as given by the Newton-Rapshon succession. The index \(j\) corresponds to the number of times that the recursive relationship in Eq. (34) is employed. The quality of the approximation for the irrational number is remarkable as shown by the figures in the fourth column.

The inclusion of this table here obeys a few reasons. The first one is related to the fact that the square root of two is an irrational number that appears in the expression of the transmission probabilities of chains with different lengths. The second, and more important, is that it manifests how difficult it is to numerically estimate if PGT is achievable in a given chain by looking at the time behavior of the transmission probabilities.

As shown in Figure 1, the PGT times necessary to achieve transmission probabilities very close to the unity are pretty short. For instance, for epsilon on the order of 0.0001, the PGT times approximately vary between 10 and 100. Shorter PGT times correspond to larger \(J_2\) values. In figure 2, we plot the transmission probabilities as functions of time in an interval that allow us to appreciate the closeness to the unity achieved by each curve. However, Figure 2 shows how difficult it is to numerically estimate if PGT is achievable in a given chain by looking at the time behavior of the transmission probabilities.

Chain with EC values that prevent the appearance of PGT

It is interesting to note that our method allows us to ascertain that we are dealing with the PGT regime and calculate explicitly the characteristic time \(t_\varepsilon\), for chains with different values of \(J_2\). Nevertheless, following a similar procedure allow us to show that there are very particular values of \(J_2\) where this kind of QST’ is forbidden.
FIG. 1: The figure shows the behavior of the PGT time $t_\varepsilon$ vs. $\varepsilon$ for $N = 4$ and different values of $J_2$ using a log–log scale. The data points corresponding to $J_2 = 1, 2, 5$ and $10$ are depicted using black, green, violet and cyan dots, respectively. The lines are included as a guide to the eye. Some of the data values are tabulated in Tables IV and VIII.

By its definition, we know that if $P(J_2; t)$ presents PGT, then it is not a periodic function of $t$. Then, periodic QST is perfect, or otherwise, the transfer is poor. Kay [4] showed that there is no PT in Heisenberg chains for $N > 2$, so periodic chains must have a bad transmission.

Periodicity in $P(J_2; t)$ is obtained for $J_2 = b/a$, where $a < b < c$ is a Pythagorean triple, $a, b, c \in \mathbb{N}$ and $a^2 + b^2 = c^2$. In this case, we obtain $\sqrt{1 + J_2^2} = c/a \in \mathbb{Q}$, and $P(b/a; t)$ is a periodic function of $t$. For the smallest Pythagorean triple, $a = 3, b = 4, c = 5 \Rightarrow J_2 = 4/3$ and $\sqrt{1 + J_2^2} = 5/3$ in Eq. (32) gives

$$P(4/3; t) = \frac{33}{100} + \frac{1}{10} \cos(4t) + \frac{9}{200} \cos\left(\frac{20t}{3}\right) - \frac{9}{40} \left(\cos\left(\frac{4t}{3}\right) + \cos\left(\frac{8t}{3}\right)\right) - \frac{1}{40} \cos(8t)$$

(35)

We obtain an upper bound for $P(4/3; t)$ replacing the cosines preceded by a plus sign by 1, and the cosines preceded by a minus sign by $-1$. Since there is always the term with $\cos(4t)$, it must be $t^*/\pi = q \delta(\varepsilon)/2$ where $q \in \mathbb{N}$ and $\delta(\varepsilon)$ is as close to 1 as we need. The arguments of the four cosine functions preceded by a minus in (32) evaluated in $t^*$ are a factor $\pi$ multiplied by

$$t_{\text{max}} = 3 \cos^{-1}\left(\sqrt{2 + \frac{3}{2}/2}\right) \approx 0.4353 \Rightarrow P(4/3; t_{\text{max}}) = 625/1024 = 0.6103515625,$$

(36)

see Fig. 3.

If $a, b, c$ are coprimes it is called a primitive Pythagorean triple (non primitive triples have the expression $(p a, p b, p c)$ where $p \in \mathbb{N}$). In this case $P(J_2 = b/a, t)$ is a periodic function of $t$, and we can prove that it does no present PGT as follows. We will see that there is no $t^*$ such that the cosine functions preceded with a plus sign approximate to 1, and those preceded by a minus sign approximate to -1. Since there is always the term with $\cos(4t)$, it must be $t^*/\pi = q \delta(\varepsilon)/2$ where $q \in \mathbb{N}$ and $\delta(\varepsilon)$ is as close to 1 as we need. The arguments of the four cosine functions preceded by a minus in (32) evaluated in $t^*$ are a factor $\pi$ multiplied by

$$\frac{(a + b + c) q \delta(\varepsilon)}{a}; \quad |(a + b - c)| \frac{q \delta(\varepsilon)}{a}; \quad |(a - b + c)| \frac{q \delta(\varepsilon)}{a}; \quad |(a - b - c)| \frac{q \delta(\varepsilon)}{a}.$$

(37)

Note that we include modules in order to have natural numbers, but the signals are not relevant. All these quantities in Eq. (37) must be close to odd numbers in order to have PGT, that is
FIG. 2: The figure shows the behavior of $P(J_2; t)$ vs. $t/\pi$ for $N = 4$, calculated using Eq. (32). The values of $P$ corresponding to $J_2 = 1, 2, 5$ and 10 are shown as black, red, green and blue continuous lines, respectively. The time interval used in the figure was selected to include some of the values of $P(J_2; \epsilon)$ tabulated in Tables IV and VII.

\begin{align}
(a + b + c) q &= (2r_{++} + 1) a ;
\end{align}

\begin{align}
|(a + b - c)| q &= (2r_{+-} + 1) a ;
\end{align}

\begin{align}
|(a - b + c)| q &= (2r_{-+} + 1) a ;
\end{align}

\begin{align}
|(a - b - c)| q &= (2r_{--} + 1) a ; \quad (38)
\end{align}

where $r_{\pm\pm}$ are natural numbers. It is known that or $a$ or $b$ is even and the other one and $c$ are odd numbers. Also we know that $a \pm b \pm c$ are even numbers, two of them $s_{1,2}$, are divisible by 4, the other two, $s_{3,4}$ are not. Then, it is clear that Eqs. (38) can not be fulfilled if $a$ is odd. If $a$ is even, then $a$ is divisible by 4, $a = 4 \tilde{a}$. For $s_3$ (or $s_4$) we have

\begin{align}
2(2l_3 + 1) q &= 4(2r_3 + 1) \tilde{a} \Rightarrow (2l_3 + 1) q = 2(2r_3 + 1) \tilde{a} \Rightarrow q = 2 \tilde{q}. \quad (39)
\end{align}

Now we use this result for $s_1$ (or $s_2$), $4(s_1/4) 2 \tilde{q} = 2(2r_1 + 1) \tilde{a}$, condition that can not be fulfilled if $a$ is odd, and so on. Therefore, we prove that PGT is absent in a numerable set of values of $J_2 = b/a$ where $a < b$ are the two smallest numbers of a primitive Pythagorean triple, and $P(J_2; t)$ is a periodic function of $t$. We will not develop the case $J_2 = a/b < 1$, which can be treated in the same way.

Then, we have a numerable set of values where there is no PGT. It is interesting to study a neighborhood of one of this isolated points. In Table IV we show values for $J_2 = 4/3 + 1/1000 = 4003/3000$ and, in Fig. 3 we compare $P(J_2; t)$ for $J_2 = 4/3$ and $4/3 + 1/1000$.

For chains of length $N = 2 \cdot 2^k$; $k > 1$ it is straightforward to see that, $\forall J_2 > 0$, $P(J_2; t)$ is not a periodic function of $t$.

Looking at Fig. 2 we can see how, when the coupling $J_2$ varies, the behavior of the transmission probability presents interesting changes. In particular, for $J_2$ large and $t \simeq n\pi/2$ with $n \in \mathbb{N}$ we see that the transmission reaches values very close to the unity. This strongly suggest that in the limit of strong coupling, we could explicitly show the appearance of PGT for particular Heisenberg spin chains. We are going to pay attention to this limit for any chain size in the next section of the present work.

### B. Chains with $N = 3 \times 2^k$ ($\alpha = 3$)

In this case, the initial condition for the recurrence equation (19) is $N = 6$ corresponding to $k = 1$, that will be calculated explicitly in the present section. For $k > 1$, we need to find the $3 \times 2^{k-1}$ eigenvalues of $A^{(N/2)}_\alpha$. In order
| $j$ | $p_j$ | $q_j$ | $P(J_2 = 4/3 + 1/1000; t_j = 1500q_j\pi)$ |
|-----|------|------|-----------------------------------|
| 1   | 5002 | 1    | 0.57264                           |
| 2   | 10005| 2    | 0.8742                            |
| 3   | 25012| 5    | 0.999992                         |
| 5   | 24716860 | 4941 | 0.999999955                        |
| 6   | 27803341 | 5558 | 0.999999982                        |
| 8   | 80323542 | 16057 | 0.9999999973                      |
| 9   | 132843743 | 26556 | 0.99999999917                      |
| 11  | 346011028 | 69169 | 0.999999999964                     |

TABLE II: Values of $p_j$, $q_j$ and $P(J_2 = 4/3 + 1/1000; t_j)$ for a spin chains with $N = 4$. The index $j$ gives the order of the continued fraction approximation for $\sqrt{25024009}$ as $p_j/q_j$. The values corresponding to orders $j = 4, 7$ and 10 do not meet the parity condition, and are not tabulated since they approximate zeros of $P(4/3 + 1/1000; t_j)$.

FIG. 3: $P(J_2; t)$ vs. $t/\pi$ calculated using Eq. (32), for a spin chain with $N = 4$. The transmission probabilities shown correspond to two particular values of the coupling $J_2$, the one linked to the lowest Pythagorean triple, $J_2 = 4/3$ and $J_2 = 4/3 + 1/1000$. The probabilities for these values of $J_2$ are shown using black and red continuous lines, respectively. The time interval selected was chosen to show the behavior of both probabilities near $t_j = 1500 \times q_j \times \pi$ with $q_j = 5$, where $P(4/3 + 1/1000, t)$ must be close to the unity, see Table II.

to simplify this task, we separate the eigenvalues given by Eq. (21) into two sets, depending on whether $(2l + 1)$ is a multiple of 3 or not,

\[
\{\lambda_{\pm}\}^{2k-1}_{2k-1} = \left\{ \pm 2 \sqrt{1 + J_2^2 + 2 J_2 \cos \left( \frac{2m + 1}{3} \pi \right) } \; ; \; m = 0, \ldots, 2k-2 - 1 \right\},
\]

which are identical to the eigenvalues of $A_{2k-1}^{(2k-1)}$, and

\[
\{\lambda_{\pm}\}^{3 \times 2k-1}_{2k-1+1} = \left\{ \pm 2 \sqrt{1 + J_2^2 + 2 J_2 \cos \left( a_3(m) \frac{\pi}{3 \cdot 2k-1} \right) } \; ; \; m = 0, \ldots, 2k-1 - 1 \right\},
\]

where $a_3(m) = ((6m + 1) - (-1)^m)/2 + 1$ represents the odd numbers that are not multiple of 3.

Using the algebraic expression of the cosine functions we obtain,
$$\{\lambda_{\pm}\}^{2k-1}_{1} = \left\{ \pm 2 \sqrt{1 + J_{2}^{2} + J_{2} \sqrt{2 \pm \sqrt{2 \pm \ldots \pm \sqrt{2}}} \right\}; \quad (42)$$

$$\{\lambda_{\pm}\}^{3 \times 2k-1}_{2k-1+1} = \left\{ \pm 2 \sqrt{1 + J_{2}^{2} + J_{2} \sqrt{2 \pm \sqrt{2 \pm \ldots \pm \sqrt{3}}} \right\}. \quad (43)$$

Now we pay attention to the simplest case, \(k = 1 \Rightarrow N = 3 \times 2^{1} = 6\) and we write the corresponding Heisenberg Hamiltonian

$$H = - (\hat{\sigma}_{1} \cdot \hat{\sigma}_{2} + J_{2} \hat{\sigma}_{2} \cdot \hat{\sigma}_{3} + \hat{\sigma}_{3} \cdot \hat{\sigma}_{4} + J_{2} \hat{\sigma}_{4} \cdot \hat{\sigma}_{5} + \hat{\sigma}_{5} \cdot \hat{\sigma}_{6}),$$

FIG. 4: The PGT time \(t_{\varepsilon}\) as a function of \(\varepsilon\) for different values of \(J_{2}\) for a chain with \(N = 6\) spins. The values of \(t_{\varepsilon}\) are calculated using the continued fraction method previously described. These values are shown as solid dots, while the lines are included as a guide. The data sets correspond to the two different possible behaviors described in the text. For \(J_{2} = 3, 5, 7, 8\) and 15 no matter how small \(\varepsilon\) is, there is a corresponding time \(t_{\varepsilon}\) such that \(1 - P/(J_{2}; t_{\varepsilon}) < \varepsilon\). For \(J_{2} = 6\) and 10 (green and brown dots, respectively) it does not matter how well the continued fraction method approximates the irrational numbers involved in the calculation of \(P\). Even for larger and larger values of the time obtained from the Dirichlet’s approximation method the respective values of \(\varepsilon\) remain without decreasing their value.

We can obtain algebraic expressions for all the eigenvalues and eigenvectors of this Hamiltonian. We also can compute, analytically, the localization of all the eigenstates in any site \((i)\) of the spin chain.
It is worth pointing out that the theorems that affirm that in chains such that \( N = 2^k \) PGT is achievable, assume that the chains have homogeneous exchange couplings coefficients. Applying the algorithm already described to find rational approximations for irrational numbers, we show numerical evidence that in chains with \( N = 3 \times 2^k \) PGT can be achieved by selecting appropriate values for \( J_2 \).

Figure 4 shows the values of the PGT time, \( t_\varepsilon \), for a chain with six spins and different values of the coupling \( J_2 \). As the data show, if \( J_2 \) is chosen as an odd integer bigger than one, the algorithm finds PGT times for arbitrarily small values of \( \varepsilon \). On the other hand, for even values of \( J_2 \), it is not possible to reach arbitrarily close to \( P = 1 \), no matter how long the arrival times considered are. See the vertical lines joining the successive approximations found by the algorithm for the irrational numbers involved in the formula of \( P(t) \) for \( N = 6 \). The green and brown vertical lines correspond to \( J_2 = 5 \) and 10. The algorithm used to find the required approximations for the irrational numbers is inefficient computationally, so obtaining PGT times larger than 10 becomes quite expensive. This restricted the values of \( \varepsilon \) that can be obtained numerically.

We fitted the data corresponding to odd values of \( J_2 \) with a power-law resulting in an exponent equal to the unity. As we will show, this result is consistent with the exponents calculated for chains \( N = 2^k \) and sits between the exponents for \( N = 4 \) and \( N = 8 \).

C. Chains with \( N = 5 \times 2^k \) (\( \alpha = 5 \))

In this section we will calculate the cases corresponding to \( N = 5 \times 2^k \). The initial condition, corresponding to \( k = 1 \) is \( N = 10 \), for \( k > 1 \), the eigenvalues of \( A_{(5 \times 2^{k-1})} \), given by Eq. (21) are, as before, divided in two sets,

\[
\{\lambda_{\pm}\}_{1}^{2^{k-1}} = \left\{ \pm 2 \sqrt{1 + J_2^2} + 2 J_2 \cos \left( \frac{(2m + 1)\pi}{2^{k-1}} \right) ; \ m = 0, \ldots, 2^{k-2} - 1 \right\},
\]

which, as the case \( \alpha = 3 \), are identical to the eigenvalues of \( A_{(2^{k-1})} \), and

\[
\{\lambda_{\pm}\}_{2^{k-1}+1}^{5 \times 2^{k-1}} = \left\{ \pm 2 \sqrt{1 + J_2^2} + 2 J_2 \cos \left( \frac{a_5(m)\pi}{5 \cdot 2^{k-1}} \right) ; \ m = 1, \ldots, 2^k \right\},\]

where

\[
a_5(m) = (10m - 9 - (-1)^m + (1 - i)^m + (1 + i)^m)/4 + 1, \ i = \sqrt{-1},
\]

represents the odd numbers that are not multiples of 5. Replacing the cosine functions by their algebraic expression we obtain,

\[
\{\lambda_{\pm}\}_{1}^{2^{k-1}} = \left\{ \pm 2 \sqrt{1 + J_2^2 + 2 J_2 \sqrt{2 \pm \sqrt{2 \pm \ldots \pm \sqrt{2}}} \right\};
\]

\[
\{\lambda_{\pm}\}_{2^{k-1}+1}^{3 \times 2^{k-1}} = \left\{ \pm 2 \sqrt{1 + J_2^2 + J_2 \sqrt{2 \pm \sqrt{2 \pm \ldots \pm \sqrt{2+\sqrt{5}}} \right\}.
\]

where \( m = 1, \ldots, 2^k \). It is possible to write the eigenvalues, eigenvectors and even the transmission probability but they are very long and complicated expressions to transcribe them in a paper.
FIG. 5: The PGT time \( t_\varepsilon \) as a function of \( \varepsilon \) for different values of \( J_2 \) for a chain with \( N = 10 \) spins. The values of \( t_\varepsilon \) are calculated using the continued fraction method previously described. These values are shown as square dots, while the lines are included as a guide. The data sets correspond to the two different possible behaviors described in the text. For \( J_2 = 5 \) and \( 11 \) no matter how small \( \varepsilon \) is there is a corresponding time \( t_\varepsilon \) such that \( 1 - P/J_2; t_\varepsilon ) < \varepsilon \). For \( J_2 = 2 \) and \( 10 \) it does not matter how well the continued fraction method approximates the irrational numbers involved in the calculation of \( P \). Even for larger and larger values of the time obtained from the Dirichlet’s approximation method the respective values of \( \varepsilon \) remain without decreasing their value.

D. Eigenvectors and localization

So far, the results presented for small chains strongly depend on the ability to produce rational approximation for the irrational numbers that appear in expressions for the transmission probabilities involving the difference between eigenvalues. Nevertheless, we have paid little attention to the behavior of the eigenvectors and its components.

For the examples analyzed the role of the eigenvectors is not as relevant as a good approximation for the eigenvalues differences, even in the case when the value of \( J_2 \) prevents the appearance of PGT. In Appendix B we analyze some properties of the eigenvectors of short spin chains.

V. PERFECT, GOOD AND PRETTY GOOD TRANSMISSION IN THE LIMIT OF STRONG COUPLING

Achieving an efficient transmission on Heisenberg spin chains is of fundamental importance for quantum technologies and related issues. Up to this point, we have studied a family of quantum spin Heisenberg chains and found analytical expressions for several quantities, in particular the transmission probabilities. It is reasonable to use these results to answer questions related to the efficient transmission of states. As shown in the previous section, it is possible to find, in some spin chains, conditions that allow for QST with high fidelity. In Fig. 2 we found some values of time for which the transmission probability between the first and last site seems to be very high. This situation occurs when the strength of the coupling \( J_2 \) is large enough.

We start analyzing the limit \( J_2 \to \infty \) for the \( N = 4 \) spin chain studied in Section IV.
\[ P_{\infty}(t) = \lim_{J_2 \to \infty} P(t) = \frac{1}{8} (3 + \cos(4t) - 4 \cos(2t)) = \sin^4(t). \] (47)

It is easy to check that we obtain perfect transmission (PT) in this limit for the times shown below

\[ P_{\infty}(t_{PT}) = (m - 1/2)\pi = 1; \quad P_{\infty}(t_{null}) = m\pi = 0, \] (48)

where \( m \in \mathbb{N} \). This result becomes relevant when we note that, in general, there is no PT for Heisenberg chains in the case of arbitrary finite interaction for \( N > 2 \). Therefore it results important to investigate spin chains with \( N > 4 \) in the limit of strong coupling. In order to solve our problem for any value of \( N \) we employ first order perturbation theory in \( \varepsilon = 1/J_2 \),

\[ h = h_1 + J_2 h_0 = J_2 (h_0 + \eta h_1). \] (49)

where matrices \( h_0 \) and \( h_1 \) have no free parameters. In the following we call the matrices \( h_0 \) and \( h_1 \) the zeroth and first order Hamiltonian matrix, respectively. It is important to note that, as the eigenstates are degenerated at \( \eta \to 0 \), we need to use degenerated perturbation theory.

### A. Properties of zeroth order Hamiltonian matrix

Taking the limit \( J_2 \to \infty \) in Eq. (12) we obtain, for chains with length \( N = 2n \)

\[ h_0 = \begin{pmatrix}
-n + 1 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 \\
0 & -n + 3 & -2 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 \\
0 & -2 & -n + 3 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 \\
0 & 0 & 0 & -n + 3 & -2 & 0 & \ldots & 0 & 0 & 0 \\
0 & 0 & 0 & -2 & -n + 3 & 0 & \ldots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & -n + 3 & -2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & -2 & -n + 3 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & -n + 1
\end{pmatrix} \] (50)

For this matrix holds:

i) It is bisymmetric.

ii) This matrix has \( n - 1 \) identical blocks of size \( 2 \times 2 \) with eigenvalues

\[ E_{<}^{(0)} = -n + 1; \quad E_{>}^{(0)} = -n + 5. \] (51)

and the corresponding eigenvectors are \( (1, 1)/\sqrt{2} \) and \( (1, -1)/\sqrt{2} \), and two identical one dimension blocks with eigenvalues \( E_{<}^{(0)} \).

It follows that the degeneration of these eigenvalues are:

\[ \deg_{<} = n + 1; \quad \deg_{>} = n - 1. \] (52)

We call \( S_{<} \) and \( S_{>} \) to the subspaces expanded by the eigenvectors of \( E_{<}^{(0)} \) and \( E_{>}^{(0)} \) respectively.
iii) We can find explicit expressions of the eigenvectors of $S_<$,

$$\hat{u}_1 = (1, 0, 0, 0, 0, \ldots, 0, 0) ; \quad \hat{u}_2 = \frac{1}{\sqrt{2}} (0, 1, 1, 0, 0, \ldots, 0, 0) ;$$

(53a)

$$\hat{u}_3 = \frac{1}{\sqrt{2}} (0, 0, 1, 1, 0, \ldots, 0, 0) ; \quad \hat{u}_4 = \frac{1}{\sqrt{2}} (0, 0, 0, 0, 1, 1, \ldots, 0) ;$$

(53b)

$$\hat{u}_n = \frac{1}{\sqrt{2}} (0, 0, 0, \ldots, 1, 1, 0) ; \quad \hat{u}_{n+1} = (0, 0, 0, 0, 0, \ldots, 0, 1),$$

(53c)

then the restriction of $h_0$ to $S_<$ is

$$h_0|_{S_<} = (-n + 1) \mathbb{I},$$

(54)

where $\mathbb{I}$ is the identity matrix of dimension $n + 1$. It is important to note that $|1\rangle y |N\rangle$ are eigenstates of $h_0$ in $S_<$.

Finally, the eigenvectors in the subspace $S_>$ are:

$$\hat{v}_1 = \frac{1}{\sqrt{2}} (0, 1, -1, 0, \ldots, 0, 0) ; \quad \hat{v}_2 = \frac{1}{\sqrt{2}} (0, 0, 0, 1, -1, \ldots, 0, 0) ; \ldots$$

(55a)

$$\hat{v}_{n-2} = \frac{1}{\sqrt{2}} (0, 0, \ldots, 0, 1, -1, 0, 0) ; \quad \hat{v}_{n-1} = \frac{1}{\sqrt{2}} (0, 0, 0, 0, \ldots, 0, 1, -1, 0),$$

(55b)

**B. Properties of the first order Hamiltonian matrix**

The expression for this matrix consists in $n \times 2 \times 2$ matrices in the diagonal,

$$h_1 = \begin{pmatrix}
  a_2 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 \\
  0 & a_2 & 0 & 0 & 0 & \ldots & 0 & 0 \\
  0 & 0 & a_2 & 0 & 0 & \ldots & 0 & 0 \\
  \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
  0 & 0 & 0 & 0 & 0 & \ldots & a_2 & 0 \\
  0 & 0 & 0 & 0 & 0 & \ldots & 0 & a_2
\end{pmatrix}, \quad \text{where } a_2 = \begin{pmatrix}
  -n + 2 & -2 \\
  -2 & -n + 2
\end{pmatrix}$$

(56)

For this matrix holds:

a) Is bisymmetric.

b) The restriction of $h_1$ to $S_<$, of dimension $n + 1 \times n + 1$, is

$$h_1|_{S_<} = \begin{pmatrix}
  -n + 2 & -\sqrt{2} & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 \\
  -\sqrt{2} & -n + 2 & -1 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 \\
  0 & -1 & -n + 2 & -1 & 0 & \ldots & 0 & 0 & 0 & 0 \\
  \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
  0 & 0 & 0 & 0 & 0 & \ldots & -1 & -n + 2 & -1 & 0 \\
  0 & 0 & 0 & 0 & 0 & \ldots & 0 & -1 & -n + 2 & -\sqrt{2} \\
  0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & -\sqrt{2} & -n + 2
\end{pmatrix},$$

(57)
c) The eigenvalues of \(h|_{S<}\) are

\[
E_{m+1}^{(l)} = -n + 2 + 2 \cos \left( m \frac{\pi}{n} \right) ; \quad m = 0, 1, \ldots, n .
\]  

It is possible to obtain an algebraic expression for these eigenvalues only for the same cases described for finite values of \(J_2\) as showed in Eq. \(23\).

Using the properties of \(h_0\) and \(h_1\) described in Sections \(\text{V A and V B}\), we obtain the self energies of \(h|_{S<}\) to first order in perturbation:

\[
E_i = -J_2(n-1) - n + 2 + 2 \cos \left((i-1) \frac{\pi}{n}\right) + O \left( \frac{1}{J_2} \right) ; \quad i = 1, 2, \ldots, n + 1 .
\]

At this moment we have all the ingredients in order to calculate the transmission probability in the strong coupling limit.

C. The transferred population as a function of time in the strong coupling limit

In this section we obtain a very simple formula for the the PT in strong coupling limit

\[
P_\infty(t) = \lim_{J_2 \to \infty} \left| \langle 1|e^{-i \hat{h}(J_2)t}|N \rangle \right|^2 = \sum_{i,j=1}^{n+1} (-1)^{i+j} w_i^2 w_j^2 e^{-i(E_i-E_j)t} ,
\]

where \(w_i^2\) are the square of the coefficients of the expansion for \(|1\rangle\) and \(|N\rangle\) in the eigenbasis of \(h\) in the strong coupling limit,

\[
w_i^2 = \begin{cases} 
\frac{1}{n} & \text{if } i = 1, n + 1 \\
\frac{1}{n} & \text{if } i \neq 1, n + 1 
\end{cases} .
\]

From Eqs. \(60\) and \(61\) we get that

\[
P_\infty(t) = \frac{1}{n^2} \left[ \left( \frac{1 + (-1)^n}{2} \right) \cos(2t) + \sum_{i=1}^{n-1} (-1)^i \cos(2 \cos(i \pi/n)t) \right]^2 + \left[ \frac{(-1 - (-1)^n)}{2} \sin(2t) + \sum_{i=1}^{n-1} (-1)^i \sin(2 \cos(i \pi/n)t) \right]^2 ,
\]

Now we split this equation for \(P_\infty\) for odd and even values of \(n\),

- \(n\) odd

\[
P_\infty(t) = \frac{1}{n^2} \left( \sum_{i=0}^{n-1} (-1)^i \sin \left( 2 \cos \left( \frac{i \pi}{n} \right) t \right) \right)^2 = \frac{1}{n^2} \left( \sin(2t) + 2 \sum_{i=1}^{(n-1)/2} (-1)^i \sin \left( 2 \cos \left( \frac{i \pi}{n} \right) t \right) \right)^2 .
\]
\[ n \text{ even} \]

\[
P_{\infty}(t) = \frac{1}{n^2} \left( \sum_{i=0}^{n-1} (-1)^i \cos \left( \frac{\pi}{n} i \right) \right)^2 = \frac{1}{n^2} \left( (-1)^{n/2} + \cos(2t) + 2 \sum_{i=1}^{n/2-1} (-1)^i \cos \left( \frac{\pi}{n} i \right) \right)^2.
\]

D. Non existence of perfect transfer in the strong coupling limit for chains with more than four spins

In this part of the work we will employ Eq. (63) that holds when we take \( k = 1 \) and \( \alpha \) odd in Eq. (22), which implies \( n = \alpha \) odd. There exist two conditions in order to obtain PT, one of these is \( \sin(2t_{PT}) = 1 \Rightarrow t_{PT} = (m+1/4)\pi \). It is sufficient to analyze the first term of the sum in Eq. (63) which should obey \( \cos(\pi/\alpha) \left( 2m + 1/2 \right) \pi \Rightarrow \cos(\pi/\alpha) = (2l+3)/(4m+1) \). By Niven’s Theorem \[43\] we know that \( \cos(\pi/\alpha) \) is a rational number only for \( \alpha = 1, 2 \) and 3. Then, we have proved that there is no PT for \( n > 3 \) odd. For the case \( n = 3 \) we can calculate explicitly \( P_{\infty} \):

\[
P_{\infty}(t) = \frac{16}{9} \sin^4 \left( \frac{t}{2} \right) \sin^2(t),
\]

This transmission probability has its maxima

\[
P_{\infty}(t_{max}) = 2 \left( m - 2/3 \right) \pi = P_{\infty}(t_{max}) = 2 \left( m - 1/3 \right) \pi = \frac{3}{4}; \quad m \in \mathbb{N},
\]

which is far away from the unity. The second condition, \( \sin(2t_{PT}) = -1 \), can be demonstrated in a similar way.

Now we need to check what happen in the case of \( n \) even, corresponding to \( k > 1 \). With this aim we have to use Eq. (64), but we need to study two different cases, \( n/2 \) even and \( n/2 \) odd. For the first one, must hold \( \cos(2t_{PT}) = 1 \Rightarrow t_{PT} = m\pi \). As before it is sufficient to analyze the first term of the sum in Eq. (64), \( 2 \cos \left( \frac{\pi}{\alpha} \right) t_{PT} = (2l+1)\pi \Rightarrow \cos \left( \frac{\pi}{\alpha} \right) = (2l+1)/2m \) but from Niven’s Theorem \[43\] we know that \( \cos(\pi/\alpha) \) is an irrational number for \( n \geq 4 \).

Then, we have proven that there is no PT for chains with \( N > 4 \) in the large coupling limit.

E. Pretty Good Transmission in the Large Coupling Limit

In this section we will show that Heisenberg Spin Chains with \( \alpha = 2 \) present PGT. For chains with \( \alpha \geq 3 \) it is straightforward to show, calculating explicitly from Eq. (63), that there is no PGT for \( k = 1 \). For the sake of clarity we write down the cases \( \alpha = 3 \) and \( \alpha = 5 \) with \( k = 1 \):

\[
P_{\infty}^{(N=6)}(t) = \frac{16}{9} \sin^4 \left( \frac{t}{2} \right) \sin^2(t); \quad P_{\infty}^{(N=10)}(t) = \frac{1}{25} \left( \sin(2t) - 4 \cos(\sqrt{5}t/2) \sin(t/2) \right)^2,
\]

where the maxima are far away from the unity. We will assume that there is no PGT for \( k > 1 \). We checked this assumption in several cases using numerical implementations of the corresponding analytical expressions.

For the case \( \alpha = 2 \) and arbitrary \( k \) the Eq. (64) takes the form
where the last square bracket has $2k-2$ terms corresponding to the $2k-2$ possible combinations of positive and negative signs. In order to have PGT we need a value of $t_\varepsilon$ such that the arguments of the cosine functions present in the first bracket should be as close as required to odd integers multiplied by $\pi$, and the arguments of the cosine functions contained in the second bracket should be as close as required to odd integers multiplied by $\pi$.

As before, $t_\varepsilon = q\pi$ assures that the modulus of all cosine functions are as close to he unity as we require. Dirichlet’s approximation theorem has not information about the parity of $q$ and $\{p_i\}$ but nevertheless in all the cases analyzed we have found an adequate set of integers (see tables III and VIII bellow).

It results very instructive to present explicitly the first two examples for $k = 2$ and $k = 3$ corresponding to $N = 8$ and $N = 16$, that, according to Eq. (68), the probabilities are

$$P_\infty^{(N=8)}(t) = \frac{1}{16} \left(1 + \cos(2t) - 2\cos(\sqrt{2}t)\right)^2,$$  \hspace{1cm} (69)

and

$$P_\infty^{(N=16)}(t) = \frac{1}{64} \left(1 + \cos[2t] + 2\cos[\sqrt{2}t] - 2\cos[\sqrt{2} - \sqrt{2}t] - 2\cos[\sqrt{2} + \sqrt{2}t]\right)^2.$$  \hspace{1cm} (70)

For $N = 8$, the only irrational number in Eq. (69) is $\sqrt{2}$, whose best rational approximations are given by the Newton-Rapshon succession, that have been already shown in Table IV here we tabulate the values calculated for $P_\infty$.

It is worth to remark that the only irrational number that it is necessary to approximate for the chain with $N = 8$, in the strong coupling limit, is the same that for a homogeneous chain with $N = 4$, so the asymptotic behavior of $t_\varepsilon$ for $N = 8$, in the strong coupling limit, and for $N = 4$, for finite values of $J_2$ are the same. Moreover, this says that if the dependence of $t_\varepsilon$ with $\varepsilon$ for $N = 8$ and $J_2$ small is different from that of the chains with $N = 4$ and $J_2$ small, then there must be a crossover that marks the regime change between the small $J_2$ behavior and the strong coupling limit.

For $N = 16$ we have to use the Dirichlet’s Approximation Theorem in order to approximate three irrational numbers. The first nine approximations to these numbers

$$M_j = 2^j; \; \sqrt{2} \simeq p_j/q_j; \; \sqrt{2 - \sqrt{2}} \simeq r_j/q_j; \; \sqrt{2 + \sqrt{2}} \simeq s_j/q_j; \; j = 1, 2, \ldots.$$  \hspace{1cm} (71)

and the corresponding probabilities $P_\infty$ can be observed in Table VIII see Appendix C.

At this point we can summarize our findings about the behavior of $t_\varepsilon$, in the weak and strong limit coupling, in Figure 6.
TABLE III: Values of the integer $q_j$ and the transmission probability in the strong coupling limit, $P_\infty(t_j)$, for a spin chain with length $N = 8$. The corresponding values of $p_j$ were tabulated in Table II. Note that for the last value tabulated $\epsilon = |1 - P_\infty| < 5 \times 10^{-49}$.

| $j$ | $q_j$ | $P_\infty(t_j = q_j \pi)$ |
|-----|------|--------------------------|
| 0   | 1    | 0.40                     |
| 1   | 2    | 0.863                    |
| 2   | 12   | 0.996                    |
| 3   | 408  | 0.99996                  |
| 4   | 470832 | 0.99999999997         |
| 5   | 627013566048 | 0.9999999999999999999999999999999999999999999999995 |
| 6   | 111198484434868137938112 | 0.9999999999999999999999999999999999999999999999995 |

FIG. 6: The PGT time as a function of $\epsilon$. The data in the figure was calculated for chains with lengths $N = 4, 8, 16, 32$ and $64$, which are shown using black, red, green, blue and brown dots, respectively. The data points obtained in the strong coupling limit correspond to the circular dots, while the data corresponding to finite values of $J_2$ are shown using dots with different shapes. For instance, for $N = 8$, the data for $J_2 = 5$ and $100$ are shown using red squares and triangles, respectively. The curves joining the different data points behave in the limit ($\epsilon \rightarrow 0$ can be fitted with power laws. See the text for details.

There is a number of features that can be extracted from the Figure, note that the scale is log-log. First, it is clear $t_\epsilon$ diverges asymptotically as a power law and that the power law exponent depends on the chain length, compare the behavior of the set of points that correspond to chains with $N = 4$, $N = 8$ that were obtained from chains with exchange coefficients ranging from the weak to the strong coupling limit. Second, the simpler expressions for the transferred population in the strong coupling limit allow us to obtain data for chains with length up to $N = 64$, while the region where $J_2$ does not correspond to the strong coupling limit (SCL) can not be explored so thoroughly. This is, among other traits, the more interesting information that the SCL offers, i.e. the asymptotic behavior of the PGT time in the SCL for a chain with length $2N$ is equal to the asymptotic behavior of the PGT time for chain with length $N$ in the “weak” coupling limit.

The crossover behavior between both limits, the SCL and the one that we termed weak coupling limit (WCL), can be better observed by looking at the data and curve corresponding to a chain with $N = 8$ and $J_2 = 100$. For $\epsilon$ large enough, and shorter PGT times, the curve is basically parallel to the curves corresponding to $N = 4$, while for smaller
values of $\varepsilon$, and larger values of the PGT times, the curve becomes parallel to the ones corresponding to $N = 8$, see the data shown using red dot triangles pointing upwards.

From the data shown in Figure 6, it is clear that, asymptotically, $t_\varepsilon \simeq 1/\varepsilon f(N)$, where $f(N)$ is an increasing function of $N$ in both regimes, SCL and WCL. Compelling as this results seems we have not been able to grasp the exact form of $f(N)$ in despite that the numerical values of the exponents are easily obtained by fitting the results. The exponents, for each one of the four sets of curves, seem to be $1/2, 3/2, 2$ and $3$. As it will be discussed later, it is clear that more data could be necessary to understand these features.

FIG. 7: $P$ vs. $1/J_2^2$ for a chain with $N = 8$. The transmission probability is plotted for two different times, $t = 12\pi$ and $t = 408\pi$, while the coupling $J = 2 \in [10, 10000]$. This particular interval was chosen to include two times tabulated in Table III both were calculated in the strong coupling limit.

The crossover observed in the behavior of $t_\varepsilon$ can also be studied by changing the quantity that is kept fixed and the one that changes, the PGT time and the strength of the $J_2$ coupling, respectively. In Figure 7 we show the behavior of the transmission probability $P(J_2, t_\varepsilon)$ for two different values of $t_\varepsilon$ for a chain with $N = 8$ spins.

The two probabilities shown in Fig. 7 correspond to $t = 12\pi$ and $t = 408\pi$, which are shown as continuous black and red curves, respectively. It is clear that for the shorter time the transmission probability reaches values close to the unity for $J_2 > 100$, but the actual value must not be precisely tuned in order to reach a QST with high fidelity. In contradistinction, when the PGT time considered is the larger one, the transmission probability shows several peaks that reach values close to the unity. The sharpness of the peaks indicates that the actual value of $J_2$ must be tuned with some care.

VI. DISCUSSION AND CONCLUSIONS

Although the results concerning the PGT time are obtained for chains with staggered exchange couplings, we think that the strong dependency of the PGT time with the chains length and the actual value of $\varepsilon$ could be one of the reasons behind the difficulties that have precluded so far the proper estimation of the PGT time in terms of $N$ and $\varepsilon$ found in previous works. On the other hand, the crossover observed between the SCL and the WCL is attributable to the staggered couplings that we have considered in this paper.

In the Strong Coupling Limit the biggest challenge to analyzing the behavior of larger chains, for instance, $N = 128$, is that looking for rational approximations of more and more irrational numbers with the same common denominator is computationally consuming. With a more efficient searching algorithm, the study of larger chains is, in principle, doable. In the case of the WCL, the difficulty is twofold. There are more irrational numbers to approximate, and the exact analytical expressions are exceedingly convoluted with hundreds, or thousands, of terms.

The power-law used to fit the different data sets compatible with PGT results in integer or semi-integer exponents. The values calculated are equal to $1/2, 1, 3/2, 2$, and $3$ for chains with $N=4, 6, 8, 10, 16, 32$, and $64$. The data for the last three lengths correspond to the Strong Coupling Limit. Remember that, as shown by our results, the PGT times obtained using the SCL for a chain with length $N = 2^k$ scale with $\varepsilon$ as the PGT times obtained for chains with half this length.
For larger chains, the numerical analysis is harder to implement since there are data sets with times ranging over ten orders of magnitude or more. Interestingly enough, the quality indexes of the regression performed to obtain the exponents indicate that the fittings are pretty good.

All in all, there is evidence that the exponent of the power-law is an increasing function of the chain size, but there is no indication of how to construct an analytical expression for this function.

From the point of view of the QST, the staggered option seems very appealing because of its simple architecture, and the fact that $t_\varepsilon$ at fixed values of $\varepsilon$ is a decreasing function of $J_2$. Moreover, in the SCL the scaling of $t_\varepsilon$ corresponds to a spin chain with half the actual length. Even with this definite improvement concerning the performance of homogeneous chains, reaching values of the fidelity close to the unity, say bigger than 0.995 could result in extremely long arrival times, see Figure 6, even for very short chains.

The finding of chains that show PGT with lengths $N = 3 \times 2^k$ and $N = 5 \times 2^k$ suggests that the regime is broadly accessible, with different interactions and architectures. If these chains can transfer quantum states more efficiently than the homogeneous ones deserves a deeper study.

The problem, of course, is that the time scale needed to observe PGT on homogeneous Heisenberg chains is orders of magnitude larger than the time scale considered in [1].

For intermediate chain lengths ($N$ between 16 and 64), Bose analyzed the time dependency of the fidelity in a time window that went up to 4000. That upper time is between two and ten orders of magnitude shorter than the one needed to pick up that the homogeneous Heisenberg chains, with lengths that are powers of two, effectively have pretty good transmission.

We consider our findings of the time scale needed to achieve PGT, together with the expanded family of chain lengths that support this regime, as the main contributions of the present work.

Appendix A: Expressions for the cosine functions evaluated at fractions of Pi

From inspection and direct calculation it is easy to check that:

$$\cos(\pi/2^2) = \frac{1}{2}\sqrt{2}$$

$$\cos(\pi/2^3) = \frac{1}{2}\sqrt{2 + \sqrt{2}}$$

$$\cos(\pi/2^4) = \frac{1}{2}\sqrt{2 + \sqrt{2 + \sqrt{2}}}$$

$$\cos(\pi/2^5) = \frac{1}{2}\sqrt{2 + \sqrt{2 + \sqrt{2 + \sqrt{2}}}}$$

Looking these expressions we propose

$$\cos(\pi/2^{k+1}) = \frac{1}{2}\sqrt{2 + \sqrt{2 + \sqrt{2 + \ldots + \sqrt{2}}}}.$$  \hspace{1cm} (A2)

and we can proof this using mathematical induction. We have already proved for $k = 1$ and, assuming the expression Eq. (A2) to be true, we need to prove

$$\cos(\pi/2^{k+2}) = \frac{1}{2}\sqrt{2 + \sqrt{2 + \sqrt{2 + \ldots + \sqrt{2}}}}.$$  \hspace{1cm} (A3)

with this aim we write

$$\cos(\pi/2^{k+1}) = \cos(2\pi/2^{k+2}) = 2\cos^2(\pi/2^{k+2}) - 1,$$  \hspace{1cm} (A4)
using Eq. (A2) in order to replace \( \cos(\pi/2^k+1) \) we can obtain Eq. (A3). Then, our initial statement is formally proven.

We can obtain a similar expression for the sine function using \( \cos^2(\alpha) + \sin^2(\alpha) = 1 \),

\[
\sin(\pi/2^k+1) = \frac{1}{2} \sqrt{2 - \sqrt{2 + \sqrt{2 + \ldots + \sqrt{2}}}},
\]

(A5)

### Appendix B: Localization of Eigenvectors

It is interesting to point out that the delicate tuning necessary to achieve PGT or avert it, as was shown in Section IV is, fundamentally, obtained in terms of spectral conditions. Since the transmission probabilities depend only on the first and the last eigenvectors components, when the eigenvectors are written on the site basis, it is natural to look at their behavior as function of \( J_2 \).

Using previous expressions we can also write the localization of the eigenvectors in any site \((i)\) for the \( N = 4 \) Heisenberg Spin chain. \( l_{\alpha}^{(i)} = |\langle E_{\alpha} | i \rangle|^2 \) as

\[
\begin{align*}
    l_4^{(1,2,3,4)} &= \frac{1}{4} \\
    l_4^{(1,4)} &= C_2^2 \\
    l_4^{(1,2,3,4)} &= \frac{1}{4} \\
    l_4^{(1,4)} &= C_4^2 \\
    l_2^{(2,3)} &= C_4^2 \\
    l_2^{(2)} &= C_4^2 \\
    l_4^{(1,2,3,4)} &= \frac{1}{4} \\
    l_4^{(1,4)} &= C_2^2 \\
    l_4^{(2,3)} &= C_4^2 \quad \text{(B1)}
\end{align*}
\]

In Fig. 8 we plot the localization \( l_{\alpha}^{(i)} \)

![Localization Coefficients](image)

**FIG. 8:** The localization coefficients as functions of the coupling \( J_2 \) (Eq. (B1)) for the four eigenvectors of a chain with four spins. (a) For states 1 and 4 (b) For states 2 and 3.

As expected, the \( l_{\alpha}^{(i)} \) are smooth functions of \( J_2 \). This is in agreement with interpretation that the behavior observed in Fig. 3 is owed to the fulfillment of the needed spectral conditions.

For the kind of spin chains that we considered in this work the localization probabilities in the different sites of the chain behave in the same way. For lengths large enough, there is reduced number of eigenvectors that become “localized” at the extremes of the chain. For this eigenvectors, the localization \( l_{\alpha}^{(i)} \) are increasing functions of \( J_2 \), see the red and blue curves in Fig. 9 a). The other eigenvectors are ”extended” along the chain, the functions \( l_{\alpha}^{(i)} \) of those eigenvectors become negligible at the extremes of the chain. For the extended eigenvectors, the localization in the interior of the chain are not decreasing or increasing functions of \( J_2 \), but their value slowly goes to the value \( 1/N \), see Fig. 9 b) and c), where the behavior described can be observed even when the data correspond to a spin chain with \( N = 6 \). Note that the eigenvector that is perfectly distributed along the length of the chain is depicted with the black curve, in both Fig. 8 and 9.

### Appendix C: Tables
FIG. 9: The localization coefficients as functions of the coupling $J_2$ (Eq. B1) for the four eigenvectors of a chain with six spins. (a) For states 1 and 6. (b) For states 2 and 5. (c) For states 3 and 4.

| $j$ | $p_j$ | $q_j$ | $P(J_2=1; t_j=q_j\pi/2)$ |
|-----|------|------|------------------|
| 1   | 1    | 1    | 0.5170           |
| 2   | 3    | 2    | 0.8962           |
| 3   | 7    | 5    | 0.9815           |
| 4   | 17   | 12   | 0.9968           |
| 5   | 41   | 29   | 0.99945          |
| 6   | 99   | 70   | 0.999906         |
| 7   | 239  | 169  | 0.9999838        |
| 8   | 577  | 408  | 0.9999972        |

TABLE IV: Values of $p_j$, $q_j$ and $P(1; t_j)$ for a chain with $N=4$ spins. The index $j$ gives the order of the continued fraction approximation of $\sqrt{2}$ as $p_j/q_j$.

| $j$ | $p_j$ | $q_j$ | $P(J_2=2; t_j=q_j\pi/2)$ |
|-----|------|------|------------------|
| 1   | 2    | 1    | 0.8459           |
| 2   | 9    | 4    | 0.9908           |
| 3   | 38   | 17   | 0.99949          |
| 4   | 161  | 72   | 0.999971         |
| 5   | 682  | 305  | 0.9999984        |
| 6   | 2889 | 1292 | 0.999999911      |
| 7   | 12238| 5473 | 0.9999999951     |
| 8   | 51841| 23184| 0.99999999972    |

TABLE V: Values of $p_j$, $q_j$ and $P(2; t_j)$ for a chain with $N=4$ spins. The index $j$ gives the order of the continued fraction approximation of $\sqrt{5}$ as $p_j/q_j$.

[1] S. Bose, Phys. Rev. Lett. 91, 207901 (2003).
[2] S. Bose, Contemporary Physics, 48:1, 13-30 (2007).
[3] G.M. Nikolopoulos and I. Jex (Edts.), Quantum State Transfer and Network Engineering, Springer-Verlag Berlin Heidelberg 2014.
[4] A. Kay - arxiv-1906.06223
[5] A. Kay, Int. J. Quantum Inf. 8:641 (2010).
[6] L. Banchi, G. Coutinho, C. Godsil, and S. Severini, J. Math. Phys. 58, 032202 (2017),
[7] C. M. van Bommel, arXiv:2010.06779v1
[8] A. Zwick and O. Osenda, J. Phys. A: Math. Theor. 44, 105302 (2011).
[9] Gamal Mograby, Maxim Derevyagin, Gerald V Dunne and Alexander Teplyaev, J. Phys. A Math. Theor. 54 125301 (2021).
TABLE VI: Values of $p_j$, $q_j$ and $P(J_2 = 5; t_j = q_j \pi/2)$ for a chain with $N = 4$ spins. The index $j$ gives the order of the continued fraction approximation of $\sqrt{26}$ as $p_j/q_j$.

| $j$ | $p_j$ | $q_j$ | $P(J_2 = 5; t_j = q_j \pi/2)$ |
|-----|-------|-------|-------------------------------|
| 1   | 5     | 1     | 0.4981                        |
| 2   | 51    | 10    | 0.99975                       |
| 3   | 515   | 101   | 0.9999976                     |
| 4   | 5201  | 1020  | 0.999999976                   |
| 5   | 52525 | 10301 | 0.99999999977                 |
| 6   | 530451| 104030| 0.9999999999977               |
| 7   | 5357035| 1050601| 0.999999999999978            |
| 8   | 54100801| 10610040| 0.99999999999999978         |

TABLE VII: Values of $p_j$, $q_j$ and $P(J_2 = 10; t_j = q_j \pi/2)$ for a chain with $N = 4$ spins. The index $j$ gives the order of the continued fraction approximation of $\sqrt{101}$ as $p_j/q_j$.

| $j$ | $p_j$ | $q_j$ | $P(J_2 = 10; t_j = q_j \pi/2)$ |
|-----|-------|-------|-------------------------------|
| 1   | 10    | 1     | 0.4956                        |
| 2   | 201   | 20    | 0.999985                      |
| 3   | 4030  | 401   | 0.999999962                   |
| 4   | 80801 | 8040  | 0.999999999905                |
| 5   | 1620050| 161201| 0.999999999999976             |
| 6   | 32481801| 3232060| 0.9999999999999941          |
| 7   | 651256070| 64802401| 0.99999999999999985       |
| 8   | 13057603201| 1299280080| 0.9999999999999999963     |

TABLE VIII: $N = 16$. The first nine quartets of values $p_j$, $q_j$, $r_j$, $s_j$ and $P_{\infty}(t_j = q_j \pi)$ that satisfy the parity condition. The ratios $p_j/q_j$, $r_j/q_j$ and $s_j/q_j$ are successive approximations for the irrational numbers $\sqrt{2}$, $\sqrt{2} - \sqrt{2}$ and $\sqrt{2} + \sqrt{2}$, respectively.

| $j$ | $q_j$ | $p_j$ | $r_j$ | $s_j$ | $P_{\infty}(t_j = q_j \pi)$ |
|-----|-------|-------|-------|-------|----------------------------|
| 1   | 7     | 10    | 5     | 11    | 0.7065                      |
| 2   | 48    | 68    | 36    | 87    | 0.6319                      |
| 3   | 362   | 512   | 277   | 669   | 0.9533                      |
| 4   | 2489  | 3520  | 1905  | 4588  | 0.9860                      |
| 5   | 10608 | 15002 | 8119  | 19601 | 0.9965                      |
| 6   | 227291| 321438| 173961| 419955| 0.9994                      |
| 7   | 1562648| 2209918| 1195099| 2887397| 0.9998                      |
| 8   | 2758647| 3901316| 2111302| 5097315| 0.99992                     |
| 9   | 28384580| 40141858| 21724617| 52447865| 0.99998                    |

[10] Matthias Christandl, Luc Vinet, and Alexei Zhedanov, Phys.Rev. A 96 032335 (2017)
[11] Xining Chen, Robert Mereau, and David L. Feder, Phys. Rev. A 93 012343 (2016)
[12] A. Zwick, G. A. Álvarez, J. Stolze and O. Osenda, Quantum Information and Computation 15, 0582 (2015).
[13] L. Banchi, T. J. G. Apollaro, A. Cuccoli, R. Vaia, and P. Verrucchi, Phys. Rev. A 82, 052321 (2010).
[14] L. Banchi, T. J. G. Apollaro, A. Cuccoli, R. Vaia and P. Verrucchi, New J. Phys. 13, 123006 (2011).
[15] Y. P. Kandel, H. Qiao, and J. M. Nichol, Appl. Phys. Lett. 119, 030501 (2021).
[16] F. Martins, F. K. Malinowski, P. D. Nissen, S. Fallahi, G. C. Gardner, M. J. Manfra, C. M. Marcus, and F. Kuemmeth, Phys. Rev. Lett. 119 227701 (2017).
[17] V. Kostak, G. M. Nikolopoulos, and I. Jex, Phys. Rev. A 75, 042319 (2007)
[18] D. M. Zajac, T. M. Hazard, X. Mi, E. Nielsen, and J. R. Petta, Phys. Rev. Applied 6, 054013 (2016).
[19] X. Li, Y. Ma, J. Han, Tao Chen, Y. Xu, W. Cai, H. Wang, Y.P. Song, Zheng-Yuan Xue, Zhang-qi Yin, and Luyan Sun, Phys. Rev. Applied 10, 054009 (2018)
[20] Jingfu Zhang, Gui Lu Long, Wei Zhang, Zhiwei Deng, Wenzhang Liu, and Zhiheng Lu, Phys. Rev. A 72, 012331 (2005); P. Cappellaro, C. Ramanathan, and D. G. Cory, Phys. Rev. A 76, 032317 (2007); J. Zhang, M. Ditty, D. Burgarth, C. A. Ryan, C. M. Chandrashekar, M. Laforest, O. Moussa, J. Baugh, and R. Laflamme, Phys. Rev. A 80, 012316 (2009)

[21] N. J. S. Loft et al New J. Phys. 18 045011 (2016).

[22] L. Banchi, A. Bayat, P. Verrucchi, and S. Bose, Phys. Rev. Lett. 106, 140501 (2011).

[23] P. Cappellaro, C. Ramanathan, and D. G. Cory, Phys. Rev. A 76, 032317 (2007); J. Zhang, M. Ditty, D. Burgarth, C. A. Ryan, C. M. Chandrashekar, M. Laforest, O. Moussa, J. Baugh, and R. Laflamme, Phys. Rev. A 80, 012316 (2009)

[24] Y. P. Kandel, H. Qiao, S. Fallahi, G. C. Gardner, M. J. Manfra, J. M. Nichol, Nature 573, 553 (2019).

[25] E. Baum, A. Broman, T. Clarke, N. C. Costa, J. Mucciaccio, A. Yue, Yuxi Zhang, V. Norman, J. Patton, M. Radulaski, and R. T. Scallettar, arXiv:2112.05740

[26] P. Hauke, F. M. Cucchietti, A. Müller-Hermes, M.-C. Bañuls, J. I. Cirac and M. Lewenstein, New Journal of Physics 12, 113037 (2010)

[27] D. Porras and J. I. Cirac, Phys. Rev. Lett. 92, 207901 (2004)

[28] C.-L. Hung, A. González-Tudela, J. I. Cirac, and H. J. Kimble, PNAS 113, 4946 (2016)

[29] X. Wang, D. Burgarth, and S. Schirmer, Phys. Rev. A 94, 052319 (2016).

[30] D. Burgarth, K. Maruyama, M. Murphy, S. Montangero, T. Calarco, F. Nori, and M. Plenio, Phys. Rev. A 81, 040303(R) (2010).

[31] S. Yang, A. Bayat, S. Bose, Phys. Rev. A 82, 022336 (2010).

[32] X.P. Zhang, B. Shao, S. Hu, J. Zou, L.A. Wu, Ann. Phys. 375 (2016) 435–443.

[33] U. Farooq, A. Bayat, S. Mancini, S. Bose, Phys. Rev. B 91, 134303 (2015).

[34] D. S. Acosta Coden, S. S. Gómez, A. Ferrón, O. Osenda, Physics Letters A 387, 127009 (2021).

[35] V. Jurdjevic and H. J. Sussmann, J. Diff. Eqn. 12, 313 (1972).

[36] D. Burgarth, S. Bose, C. Bruder, and V. Giovannetti, Phys. Rev. A 79, 060305(R) (2009).

[37] V. Ramakrishna, M. V. Salapaka, M. Dahleh, H. Rabitz, and A. Peirce, Phys. Rev. A 51, 960 (1995).

[38] Vincent X. Genest, Luc Vinet, Alexei Zhedanov, Annals of Physics 371 (2016) 348–367

[39] Vinet, Zhedanov, Physics Letters A 431 (2022) 127973

[40] P. Serra, A. Ferrón and O. Osenda, Pretty good quantum state transfer on isotropic and anisotropic Heisenberg spin chains with tailored site dependent exchange couplings, arXiv:2112.05512 [quant-ph]

[41] A. Ferrón, P. Serra and O. Osenda, Understanding the propagation of excitations in quantum spin chains with different kind of interactions, arXiv:2112.15512 [quant-ph]

[42] M. Mouri, Bisymmetric, Persymmetric Matrices and Its Applications in Eigendecomposition of Adjacency and Laplacian Matrices, JIMCS 6, 766 (2012).

[43] I. Niven, Irrational Numbers, in Carus Mathematical Monographs, Number 11, 1956.