PHYSICAL REVIEW A **86**, 052319 (2012)

Almost perfect state transfer in quantum spin chains

Luc Vinet
Centre de recherches mathématiques Université de Montréal, P.O. Box 6128, Centre-ville Station, Montréal (Québec), Canada H3C 3J7

Alexei Zhedanov
Institute for Physics and Technology, R. Luxemburg Strasse 72, 83114 Donetsk, Ukraine
(Received 21 May 2012; revised manuscript received 22 October 2012; published 19 November 2012)

The natural notion of almost perfect state transfer (APST) is examined. It is applied to the modeling of efficient quantum wires with the help of XX spin chains. It is shown that APST occurs in mirror-symmetric systems, when the 1-excitation energies of the chains are linearly independent over rational numbers. This result is obtained as a corollary of the Kronecker theorem in Diophantine approximation. APST happens under much less restrictive conditions than perfect state transfer and moreover accommodates the unavoidable imperfections. Some examples are discussed.

DOI: 10.1103/PhysRevA.86.052319 PACS number(s): 03.67.Hk

I. INTRODUCTION

The design of models to transfer quantum states between distant locations is of relevance to many quantum information protocols. In recent years, spin chains have been proposed [1,2] as possible basic systems in the construction of such quantum channels. In these devices, the state of the qubit at one end of the chain is transferred to the qubit at the other end after some time. A key advantage of this method is that it minimizes the need for external interventions as the transfer is realized through the intrinsic dynamics of the chain.

The efficiency and reliability of quantum wires must be high. Ideally, it is wished that the probability of finding the initial state as the output be 1; when this is so, one speaks of perfect state transfer (PST). It has been shown, in particular, that PST can be achieved in spin chains by properly engineering and modulating the couplings between the sites [2,3].

In this context, a question of practical importance is that of the robustness of these ideal transfer properties in view of the unavoidable manufacturing and experimental deviations from the theoretical specifications.

There are many sources of errors: nonsynchronous or imperfect input and readout operations, fabrication defects, additional interactions, systematic biases, etc. What their influences on the fidelity of state transfer are [4,5] and how to correct or circumvent them [6,7] has been the object of various studies. We here relate particularly to the errors imputable to the quantum wires and measurements. In [8] (see also [9,10]) the imperfections in the production of the device are modeled by adding random perturbations to the couplings and magnetic fields of a chain with PST. In [11] (which uses methods similar to those in [12] and [13]), modulated chains are coupled to boundary states to make transfer more robust against imperfections which are also randomly simulated. We adopt in the following a complementary approach.

We take for given that the manufacturing of the chains will not be perfect and that the precise PST requirements will not be met. Notionally, we assume that the imperfections are static. We then consider under which conditions will state transfer be almost perfect. In other words, instead of examining the effect of perturbations on PST chains, we readily attempt to characterize the chains that somehow incorporate defects and come "very" close to achieving PST.

The simplest spin chains exhibiting PST are governed by XX Hamiltonians with nearest-neighbor interactions. We confine ourselves to these systems in the following. Given that the total spin projection commutes with the Hamiltonians, many of the state transfer properties can be obtained by focusing on the 1-excitation sector of the state space. The corresponding restrictions of the Hamiltonians are tridiagonal Jacobi matrices J whose entries are the couplings and magnetic fields of the chains. Naturally, these J are diagonalized by orthogonal polynomials (OPs). The perfect transfer of a single spin up from one end of the chain to the other is possible only if J is mirror symmetric; moreover, it puts strong requirements on its spectrum. The theory of OPs is very useful to obtain these results.

The same framework is adopted to determine the conditions for almost perfect state transfer (APST). The question now is this: Under what circumstances are there times for which the transition probabilities from one site to another can be made to approach 1? Mirror symmetry will again be necessary, as we shall see. It is sufficient, however, for the spectrum of a mirror-symmetric J to obey conditions much milder than in the PST case. Interestingly, these results will follow from the Kronecker theorem in Diophantine approximation.

The remainder of the paper proceeds as follows. We first review in Sec. II how 1-excitation state transfer is realized in XX spin chains and how the eigenstates are obtained with the help of OPs. Almost perfect state transfer is defined in Sec. III and necessary and sufficient conditions for its occurrence are determined. In Sec. IV, it is shown how various chains with APST can be obtained from a parent chain with APST through a procedure referred to as spectral surgery [13]. Section V offers a number of illustrative examples: situations where APST occurs and cases where neither PST nor APST are possible. In a significant model, the times for which APST is attained can be estimated showing in this instance that a good approximation to PST is obtained in finite time independently of the size of the chain.

Let us finally draw attention to recent related and complementary publications that have made use of the same tools from number theory in the case of spin chains with

 ©2012 American Physical Society

uniform couplings. In his thesis [14], using the Kronecker theorem, Burgarth has shown that the Heisenberg XX spin chains with prime lengths have arbitrary good fidelity. In [15], Godsil introduced the notion of pretty good state transfer on graphs, which is equivalent to our definition of APST. Our terminology is dictated by the fact that in these instances the transition amplitudes are almost periodic functions. Recently, the characterization of the uniform XX Heisenberg chains which admit this pretty good state transfer was analyzed using again number theoretic methods [16].

In dealing with the Heisenberg XX spin chain with uniform coupling and zero magnetic fields, the mirror-symmetry of the one-excitation Hamiltonian is *de facto* ensured as this operator coincides with the adjacency matrix of the $(N+1)$ path. As will be seen, this symmetry requirement comes into play in relation with APST, when more general couplings and magnetic fields are considered. It is remarked in [15] that in order to get a good approximation to PST, the waiting time must be very large. Numerical results presented in [16] indicate that for a given level of fidelity, or approximation, the required times grow linearly with N, the number of sites in the chain minus one. (We comment on these observations in Sec. V, using exact results on almost perfect return [17] as applied to the uniform XX chain.) Thus, Godsil [15] expressed the view that pretty good state transfer or APST is not a satisfactory substitute for PST in practice. We here wish to stress in this connection that when considering nonuniform couplings, there are situations, as shown by an aforementioned example in Sec. V, where high fidelity can be achieved in finite time irrespectively of the chain length. This suggests that the class of spin chains with APST, a much larger one than the PST family, should not be so radically deemed of impractical use at this point.

II. 1-EXCITATION STATE TRANSFER IN XX SPIN CHAINS

We consider XX spin chains with nearest-neighbor interactions. Their Hamiltonians H are of the form

$$H=\frac{1}{2}\sum_{l=0}^{N-1}J_{l+1}\left(\sigma_l^x\sigma_{l+1}^x+\sigma_l^y\sigma_{l+1}^y\right)+\frac{1}{2}\sum_{l=0}^{N}B_l\left(\sigma_l^z+1\right), \tag{2.1}$$

where J_l are the constants coupling the sites $l-1$ and l and B_l are the strengths of the magnetic field at the sites l ($l=0,1,\dots,N$). The symbols σ_l^x, σ_l^y, σ_l^z stand for the Pauli matrices which act on the lth spin.

It is immediate to see that

$$\left[H,\frac{1}{2}\sum_{l=0}^{N}\left(\sigma_l^z+1\right)\right]=0,$$

which implies that the eigenstates of H split in subspaces labeled by the number of spins over the chain that are up. In order to characterize the chains with APST, it suffices to restrict H to the subspace spanned by the states which contain only one excitation. A natural basis for that subspace is given by the vectors

$$|e_n\rangle=(0,0,\dots,1,\dots,0),\quad n=0,1,2,\dots,N,$$

where the only "1" occupies the nth position. The restriction J of H to the 1-excitation subspace acts as follows:

$$J|e_n\rangle=J_{n+1}|e_{n+1}\rangle+B_n|e_n\rangle+J_n|e_{n-1}\rangle. \tag{2.2}$$

Note that

$$J_0=J_{N+1}=0 \tag{2.3}$$

is assumed.

Consider the polynomials $\chi_n(x)$ obeying the recurrence relation

$$J_{n+1}\chi_{n+1}(x)+B_n\chi_n(x)+J_n\chi_{n-1}(x)=x\chi_n(x), \tag{2.4}$$

with

$$\chi_{-1}=0,\quad \chi_0=1. \tag{2.5}$$

They satisfy the orthogonality relations

$$\sum_{s=0}^{N}w_s\chi_n(x_s)\chi_m(x_s)=\delta_{nm}, \tag{2.6}$$

where w_s are the discrete weights taken to satisfy

$$\sum_{s=0}^{N}w_s=1. \tag{2.7}$$

In what follows we take the eigenvalues x_s in increasing order:

$$x_0<x_1<x_2<\cdots<x_N. \tag{2.8}$$

Let

$$|x_s\rangle=\sum_{n=0}^{N}\sqrt{w_s}\chi_n(x_s)|e_n\rangle. \tag{2.9}$$

It is easily seen that these vectors $|s\rangle$ are eigenstates of J with eigenvalues x_s

$$J|x_s\rangle=x_s|x_s\rangle. \tag{2.10}$$

Since both bases $\{|s\rangle\}$ and $\{|e_n\rangle\}$ are orthonormal,

$$\langle e_n|e_m\rangle=\delta_{nm},\quad \langle x_{s'}|x_s\rangle=\delta_{ss'},$$

we also have

$$|e_n\rangle=\sum_{s=0}^{N}\sqrt{w_s}\chi_n(x_s)|x_s\rangle. \tag{2.11}$$

Let $P_{N+1}(x)$ be the characteristic polynomial of J:

$$P_{N+1}(x)=(x-x_0)(x-x_1)\cdots(x-x_N). \tag{2.12}$$

The discrete weights are expressed as [18]

$$w_s=\frac{h_N}{P_N(x_s)P'_{N+1}(x_s)},\quad s=0,1,\dots,N, \tag{2.13}$$

with $h_N=J_1^2J_2^2\cdots J_N^2$ and $P_N(x)=h_N^{1/2}\chi_N(x)$.

III. NECESSARY AND SUFFICIENT CONDITIONS FOR ALMOST PERFECT QUANTUM STATE TRANSFER

By APST we mean the following.

Assume that the spin chain is prepared at time $t=0$ in the pure state $|e_0\rangle$. This means that that at site $n=0$ the spin is up while all other spins are down.

For arbitrary times t, this state will evolve into the state

$$|e_0(t)\rangle = e^{-itJ}|e_0\rangle. \quad (3.1)$$

We demand that for any small $\epsilon > 0$, there exists a value of time t such that

$$||e_0(t)\rangle - e^{i\phi(t)}|e_N\rangle|^2 < \epsilon, \quad (3.2)$$

where $\phi(t)$ is a real parameter which can depend on t. This means that the state $|e_0(t)\rangle$ can be as close to the state $|e_N\rangle$ as desired and that $|e_0\rangle$ has thus undergone at time t an almost perfect transfer.

The notation $|\eta - \xi|^2$ for two vectors ξ and η stands, as usual, for

$$|\xi - \eta|^2 = \sum_{k=0}^{N} |\xi_k - \eta_k|^2, \quad (3.3)$$

where ξ_k are the expansion coefficients of the vector ξ over a basis, say $|e_k\rangle$:

$$\xi = \sum_{k=0}^{N} \xi_k |e_k\rangle. \quad (3.4)$$

Recall that the condition for 1-excitation PST reads

$$|e_0(t)\rangle = e^{-i\phi(t)}|e_N\rangle; \quad (3.5)$$

this means that there then exists a time t for which the state $|e_0(t)\rangle$ coincides (up to a phase factor $e^{i\phi(t)}$) with the state $|e_N\rangle$.

In the case of APST, there is no time t for which condition (3.5) is verified. Nevertheless, it is possible to approach the state $|e_N\rangle$ with any prescribed degree of accuracy. From a practical point of view, there is no essential difference between perfect and APST, owing to inevitable technological and measurement errors. However, the APST conditions are much weaker than the PST ones. APST therefore widens the possibilities for constructing efficient quantum wires.

Let us first derive the necessary condition for APST.

Taking into account expansion Eq. (2.11), we have

$$|e_0(t)\rangle = \sum_{s=0}^{N} \sqrt{w_s} e^{-ix_s t}|x_s\rangle, \quad |e_N\rangle = \sum_{s=0}^{N} \sqrt{w_s}\chi_N(x_s)|x_s\rangle \quad (3.6)$$

and hence

$$|e^{-i\phi(t)}|e_0(t)\rangle - |e_N\rangle|^2 = \sum_{s=0}^{N} w_s |e^{-i\phi(t)-itx_s} - \chi_N(x_s)|^2. \quad (3.7)$$

It is easily seen that in order to fulfill condition (3.2) we need

$$|\chi_N(x_s)| = 1. \quad (3.8)$$

To convince oneself of this fact, suppose that (3.8) does not hold and assume that for some $s = 0,1,\ldots,N$, we have $\chi_N(x_s) = a$ with $|a| \neq 1$. In this case, using the reverse triangle inequality we have

$$|e^{-i\phi(t)-itx_s} - \chi_N(x_s)|^2 \geqslant (|a| - 1)^2 > 0$$

and as a consequence the right-hand side of (3.2) cannot be made arbitrarily small.

Since $\chi_N(x)$ has only real coefficients (3.8) implies that $\chi_N(x_s) = \pm 1$. From general properties of OPs [13,18] it follows, using (2.12), that (3.8) amounts to

$$\chi_N(x_s) = (-1)^{N+s}. \quad (3.9)$$

As shown in [13], Eq. (3.9) implies that the matrix J is persymmetric, or mirror-symmetric, that is,

$$RJR = J, \quad (3.10)$$

where R is the reflection matrix

$$R = \begin{pmatrix} 0 & 0 & \ldots & 0 & 1 \\ 0 & 0 & \ldots & 1 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 1 & 0 & \ldots & 0 & 0 \end{pmatrix}.$$

We have thus obtained a necessary condition for APST, namely, that the Jacobi matrix J corresponding to the spin XX Hamiltonian should be mirror symmetric. This coincides with one of the necessary conditions for PST [12]. The other condition for PST requires that

$$x_{s+1} - x_s = \frac{\pi}{t} M_s, \quad (3.11)$$

where M_s are arbitrary positive odd numbers.

We now obtain the conditions on the spectrum of J for APST.

The matrix J is Hermitian and mirror symmetric with $J_i > 0$ and hence all its eigenvalues x_s are real and distinct.

Let $f_{0n}(t)$ be the amplitude for finding the system in the state $|n\rangle$ at time t if it was in the state $|e_0\rangle$ at time $t = 0$,

$$f_{0n}(t) = \langle e_n|e^{-iJt}|e_0\rangle. \quad (3.12)$$

It is easily seen that [13]

$$f_{0N}(t) = \sum_{s=0}^{N} w_s e^{-ix_s t}\chi_N(x_s). \quad (3.13)$$

Taking into account (3.9) we have

$$f_{0N}(t) = \sum_{s=0}^{N} w_s e^{-ix_s t}(-1)^{N+s}. \quad (3.14)$$

Mindful of the normalization (2.7), it is seen that condition $|f_{0N}(t)| \approx 1$ is equivalent to the condition that

$$e^{-ix_s t}(-1)^{N+s} \approx e^{i\phi} \quad (3.15)$$

for a fixed value t, where $\approx$ means "approximately equal with any prescribed accuracy." To paraphrase (3.15), there thus should be a value t of time for which the left-hand side is as close as desired to a phase independent of s.

This means that $|f_{0N}(t)|$ is an almost periodic function.

Recall that any almost periodic function $f(t)$ is a formal trigonometric series [19]

$$f(t) = \sum_{n=-\infty}^{\infty} a_n e^{i\omega_n t}, \quad (3.16)$$

where ω_n are real parameters. For periodic functions $f(t + T) = f(t)$, one has $\omega_n = \frac{2\pi n}{T}$ and (3.16) is the ordinary Fourier series. For almost periodic functions there exist the so-called almost periods. This means that for every $\varepsilon > 0$ there exists a real parameter $T = T(\varepsilon)$ such that the inequality

$$|f(t+T) - f(t)| < \varepsilon \tag{3.17}$$

holds for all t.

In turn, condition (3.15) is tantamount to an inequality involving the exponents that can be stated as follows.

For every $\delta > 0$ there exist a real parameter ϕ and a value of time t such that

$$|x_s t - \pi s + \phi| < \delta \pmod{2\pi}. \tag{3.18}$$

In more detail, Eq. (3.18) can be rewritten in the form

$$-\delta < x_s t - \pi s + \phi + 2\pi M_s < \delta, \tag{3.19}$$

where M_s are integers which may depend on s.

This obviously amounts to a condition on the spectrum of J for APST to occur. The question is as follows. What are the properties that the eigenvalues x_s must possess to ensure that it is possible to find a time t and integers M_s so that (3.19) is satisfied and hence APST is realized. In other words, given the set of real numbers $a_s = \phi - \pi s$, this is asking the following: When is it possible to find values of t for which $x_s t$ is approximated in terms of integers by $a_s - 2\pi M_s$ with any prescribed accuracy?

The solution of this Diophantine approximation problem (3.19) is given remarkably by the Kronecker theorem [20,21].

In order to state it, let us introduce the following definition [20,21]: A set $\alpha_i, i = 1,2,\ldots,$ of real numbers is called linearly independent if for any n the only rational values of $r_1,\ldots,r_n$ satisfying

$$r_1\alpha_1 + r_2\alpha_2 + \cdots + r_n\alpha_n = 0$$

are $r_1 = r_2 = \cdots = r_n = 0$.

The Kronecker theorem can be formulated in two versions, one a special case of the other. The first version is attributed to Kronecker himself.

Version 1. Assume that the real numbers x_s, $s = 0,1,\ldots,N$ are linearly independent over the field of rational numbers. Let $a_0, a_1, \ldots, a_N$ be fixed arbitrary real numbers. The Kronecker theorem states that for every $\delta > 0$ there exist a real t and integers $M_0, M_1, \ldots, M_N$ such that the inequalities

$$|x_s t - a_s - 2\pi M_s| < \delta, \quad s = 0,1,2,\ldots,N \tag{3.20}$$

hold.

We see how this theorem directly applies to the APST problem. Indeed, provided that the eigenvalues are linearly independent over the rational numbers, we may conclude from the Kronecker theorem that for every parameter ϕ it is possible to find a time t so that $|f_{0N}(t)|$ is as close to 1 as desired.

In many cases, however, the eigenvalues x_s are not linearly independent. This means that there can exist L independent relations of the type

$$r_0^{(i)} x_0 + r_1^{(i)} x_1 + \cdots + r_N^{(i)} x_N = 0, \quad i = 1,2,\ldots,L \leqslant N, \tag{3.21}$$

where $r_s^{(i)}$ are integers such that for every $i = 1,2,\ldots,L$ at least one of them is nonzero. (The use of integers is equivalent to that of rationals and more practical.)

When additional relations such as (3.21) are present, the Kronecker theorem can be formulated as follows [21].

Version 2. Assume that the real parameters x_s, $s = 0,1,\ldots,N$ are all distinct and moreover that there are L relations of the type (3.21) with nontrivial sets $\{r_0^{(i)},\ldots r_N^{(i)}\}$ of integers.

Then, the approximation condition (3.20) holds for every $\delta > 0$ if and only if the real quantities a_i satisfy the conditions

$$r_0^{(i)} a_0 + r_1^{(i)} a_1 + \cdots + r_N^{(i)} a_N \equiv 0 \pmod{2\pi}, \quad i = 1,2,\ldots,L \tag{3.22}$$

with the same integers $r_i^{(i)}$ as in (3.21).

For the proof of this statement, see [21].

Using this (generalized) version of the Kronecker theorem, we can formulate the necessary and sufficient conditions for APST.

General result. Let $x_0, x_1, \ldots, x_N$ be $N+1$ distinct eigenvalues of the Jacobi matrix J corresponding to the XX spin chain (2.1). Assume that there are $L \leqslant N$ relations of the type (3.21) with nonzero integer parameters $r_s^{(i)}$.

Then, the following conditions are necessary and sufficient for APST:

(i) the Jacobi matrix J is mirror-symmetric, that is,

$$B_s = B_{N-s},\ J_s = J_{N+1-s}, \quad s = 0,1,\ldots,N; \tag{3.23}$$

(ii) the L linear relations

$$\sum_{s=0}^{N} r_s^{(i)}(\pi s - \phi) = 0 \pmod{2\pi}, \quad i = 1,2,\ldots L \tag{3.24}$$

are compatible.

An obvious special case of this statement occurs when all eigenvalues x_s are linearly independent over the field of rational numbers. This means that $L = 0$, that is, that there are no additional relations such as (3.24) and that version 1 of the Kronecker theorem suffices to conclude to the occurrence of APST. In such instances, we see that the mirror symmetry of J and the linear independence of the eigenvalues represent the necessary and sufficient conditions for APST.

Let us now compare the conditions for APST with the conditions for PST. It is known that the PST conditions are [12]

(i) the Jacobi matrix J is mirror symmetric;

(ii) assuming that the eigenvalues x_s are ordered so that $x_0 < x_1 < \cdots < x_N$, the differences $\Delta_s = x_{s+1} - x_s$ are proportional to odd numbers:

$$\Delta_s = \kappa(2j_s + 1), \tag{3.25}$$

where j_s are integers and κ is a constant not depending on s.

We see that mirror-symmetry is necessary for both PST and APST. This implies that the matrix J and hence the Hamiltonian can be uniquely reconstructed from the eigenvalues $x_0, x_1, \ldots, x_N$ when either process occurs. Indeed, since (3.9) (which implies mirror-symmetry) specifies $\chi_N(x)$ at $N+1$ distinct points, this polynomial can be obtained by Lagrange interpolation. Two OPs associated to the three-diagonal matrix J are therefore known: $\chi_N(x)$ and the characteristic polynomial $\prod_{s=0}^{N}(x - x_s)$ of degree $N+1$. As shown in [13], all the OPs can then be found by the Euclidean algorithm, thereby providing their three-term recurrence relation explicitly, that is, giving all the couplings J_i and magnetic fields B_i.

The difference in the conditions for PST and APST arises only in the restrictions on the spectrum or the eigenvalues of J. As is observed, these conditions are much more stringent for PST than for APST.

IV. SPECTRAL SURGERY AND APST

A spectral surgery procedure was proposed in [13] as a way to construct XX spin chains with PST from such systems already known to possess the PST property.

Given the initial spectrum $X_N = \{x_0, x_1, \ldots, x_N\}$, under spectral surgery, one or several levels $x_{i_1}, x_{i_2}, \ldots, x_{i_j}$ are removed from the set X_N.

The reduced set is $\tilde{X}_{N-j} = X_N \setminus R_j$, where $R_j = \{x_{i_1}, x_{i_2}, \ldots, x_{i_j}\}$ is the set of levels that have been removed. The spectral levels determine the (mirror-symmetric) Jacobi matrix J (and hence the Hamiltonian of the XX spin chain) uniquely. Thus, the new spectral set $\tilde{X}_{N-j}$ generates a new Jacobi matrix $\tilde{J}$ of dimension $(N+1-j) \times (N+1-j)$. Certain restrictions need to be imposed on the possible choices of sets R_j. Namely, R_j can contain any number of levels starting from the first one, say $R^{(0)}_{M_1} = \{x_0, x_1, \ldots, x_{M_1-1}\}$ or similarly, any number of levels from the last level, say $R^{(N)}_{M_2} = \{x_N, x_{N-1}, \ldots, x_{n-M_2+1}\}$. The only restriction is that there should be no gaps in the above sequences. Apart from these two elementary surgeries, levels can also be extracted from the middle of the spectral set X_N; in this case the requirement is the following: All such level sets should consist in the union of subsets $R^{(i)}_L = \{x_i, x_{i+1}, \ldots, x_{i+L-1}\}$ of even length L and without gaps within $R^{(i)}_L$. Equivalently, one can say that only pairs x_i, x_{i+1} of neighbor levels can be removed from the middle of the set X_N.

Remarkably, the Jacobi matrix $\tilde{J}$ corresponding to a surgered set $\tilde{X}_{N-j}$, is obtained from the initial Jacobi matrix by j Christoffel transforms (see [13] for details).

That is, after j Christoffel transforms, we obtain a new Jacobi matrix $\tilde{J}$ which is mirror-symmetric and satisfy the PST property. This observation makes it possible to generate new explicit examples with PST without the need to perform the inverse spectral problem algorithm. This is advantageous since the formulas of the Christoffel transform are rather simple.

One such example was already given in [13]. Let N be odd. We start with the uniform grid $X_N = \{-N/2, -N/2+1, \ldots, N/2\}$ and then remove $2L$ levels symmetrically from the middle of the set X_N

$$X_{N-2L} = \{-N/2, -N/2+1, \ldots -L-3/2, -L-1/2, \\ L+1/2, L+3/2, \ldots, N/2-1, N/2\}. \quad (4.1)$$

Such a spectral set corresponds to the model of the XX spin chain with PST proposed in [22].

Consider what the effect of spectral surgery is with respect to APST.

It is almost obvious that under an arbitrary admissible surgery procedure the APST property survives. Indeed, if all eigenvalues x_i were linearly independent over the field of rational numbers, then any reduced set $\tilde{X}_{N-j}$ will obviously satisfy the same property.

Assume that there exists a set of linear relations (3.21) on the spectral levels x_s. APST is possible if and only if the set of linear relation (3.24) is compatible (it is assumed *a priori* that the matrix J is mirror symmetric).

Under spectral surgery some levels of the set X_N are removed. This means that some of relations (3.21) will disappear (or remain the same). This implies that the new Jacobi matrix $\tilde{J}$ will also possess APST.

Interestingly, this method can sometimes generate a chain with APST, even if the initial chain lacks this property. Indeed, the absence of APST for a given mirror-symmetric XX chain means that relations (3.24) are incompatible. When we remove some of the levels x_i the number of relations (3.21) can be reduced, which, in principle, can lead to the compatibility of the reduced set of relations (3.24). Of course, one should seek to realize this in concrete examples. We plan to investigate this problem in the future.

V. EXAMPLES AND SPECIAL CASES

We present a number of examples and special cases in this section.

(i) We indicate how the central result specializes in the absence of magnetic fields.

(ii) We record the circumstances for APST in the uniform XX chain and discuss the relation between the waiting time and the length of the chain for this particular system, using results on almost perfect return (to the point of origin).

(iii) We show, not too surprisingly, that the conditions for PST are a special case of the conditions for APST.

(iv) We consider in detail the case $N=4$ corresponding to spin chains with five sites. In this instance, it is possible to give a very explicit analysis of APST and to estimate waiting times using standard methods of Diophantine approximation. The conditions for all the possible cases (PST, APST, and neither) are derived.

(v) We introduce a remarkable model based on the para-Krawtchouk polynomials that can exhibit PST, APST, or neither depending on the value of one of its parameters; it will furthermore be seen that the waiting times can be estimated and found to be finite independently of the size of the chain for arbitrarily good fidelities in some special APST situations.

A. Absence of magnetic fields

Consider the special situation corresponding to zero magnetic fields $B_s = 0$. In this case the Jacobi matrix J has only two nonzero diagonals. The corresponding OPs are symmetric $P_n(-x) = -P_n(x)$ and hence the eigenvalues satisfy the properties

$$x_s + x_{N-s} = 0, \quad s = 0, 1, \ldots, N, \quad (5.1)$$

where it is assumed that $x_0 < x_1 < \cdots x_N$.

Consider first the case N odd. Then one has $(N+1)/2$ independent relations (5.1) for $s = 0, 1, \ldots, (N-1)/2$. They coincide with relations (3.21) where only two integers are nonzero and given by $r_s = r_{N-s} = 1$.

Relations (3.24) then reduce to the single condition

$$\pi N - 2\phi = 0 \pmod{2\pi}, \quad (5.2)$$

from which we find

$$\phi = \begin{cases} -\pi/2 & \text{if} \quad N = 4m+3 \\ \pi/2 & \text{if} \quad N = 4m+1 \end{cases} \pmod{2\pi}. \tag{5.3}$$

If one assumes that the eigenvalues $x_0, x_1, \ldots, x_{(N-1)/2}$ are linearly independent, then the Kronecker theorem guarantees with $\phi = \pm\pi/2$ that the corresponding spin chain will exhibit APST.

If N is even, we shall have the $N/2$ independent relations (5.1) for $i = 0,1,\ldots,N/2-1$ and in addition

$$x_{N/2} = 0. \tag{5.4}$$

Conditions (3.24) are compatible if and only if

$$\phi = \begin{cases} 0 & \text{if} \quad N/2 \quad \text{is even} \\ \pi & \text{if} \quad N/2 \quad \text{is odd} \end{cases} \pmod{2\pi}. \tag{5.5}$$

Again, if the eigenvalues $x_0, x_1, \ldots, x_{N/2-1}$ are linearly independent, the APST property is present.

B. The uniform XX chain with zero magnetic fields

The APST (or pretty good state transfer) of the XX chain with uniform couplings and no magnetic fields, that is, $J_s = 1$ and $B_S = 0$ for all s, have recently been sorted out in [16]. It has been found there that a chain of length $N+1$ admits APST if and only if $N = p-2$ or $2p-2$, where p is prime or if and only if $N = 2^m - 2$. As a matter of fact, the proof of that result given in [16] effectively proceeds from the application of version 2 of the Kronecker theorem and the use of trigonometric relations between the eigenvalues

$$x_s = 2\cos[\pi s/(N+2)], \quad s = 1,2,\ldots,N+1, \tag{5.6}$$

which are given by the roots of the Chebyshev polynomials of second kind for this model.

In the same reference [16] (see also [15]), it is pointed out, on the basis of numerical analysis, that the waiting times for APST will grow with the size of the chain. This has cast doubts on the practical use of APST. Our next examples hopefully dissipate this negative view by showing that there are models exhibiting APST where the waiting times stay finite as the size is grown.

Before we leave this uniform XX chain, we would like to offer the following comment on the waiting times as the chain is taken to have very large length.

The quantity

$$f_{00}(t) = \langle e_0 | e^{-itJ} | e_0 \rangle \tag{5.7}$$

represents the return amplitude, that is, the amplitude to return to the initial (input) state after a time t. Since

$$|e^{-itJ}|e_0\rangle - e^{i\phi}|e_N\rangle| = |e^{itJ}|e_N\rangle - e^{-i\phi}|e_0\rangle|,$$

if we have APST from $|e_0\rangle$ to $|e_N\rangle$, we also have APST from $|e_N\rangle$ to $|e_0\rangle$. As a consequence, in a chain with APST, we must observe that there is almost perfect return, that is that there are times t_n, $n = 0,1,2,\ldots$, such that

$$\lim_{n\to\infty} |f_{00}(t_n)| = 1. \tag{5.8}$$

The conditions for almost perfect return have been analyzed in [17] and can be simply stated: An XX spin chain will exhibit almost perfect return if and only if its one-excitation Hamiltonian J has a pure point spectrum. As is readily seen, the spectrum of the uniform XX chain becomes continuous as N, the number of sites minus 1, becomes infinite (see [17] for more details.) It follows that almost perfect return does not occur in the case of a semi-infinite Heisenberg XX chain and hence not surprisingly an infinite time is required for APST in this model.

C. PST as a special case of APST

If a set $\{x_0, x_1, \ldots, x_N\}$ of eigenvalues satisfies the APST conditions, it is clear that the affine transformed eigenvalues $\tilde{x}_s = \alpha x_s + \beta$ will also satisfy the APST conditions. In particular, we can always assume that $x_0 = 0$ and $x_1 = 1$. The PST condition (3.25) then implies that $x_{2s} = K_{2s}$ are even integers while $x_{2s+1} = K_{2s+1}$ are odd integers. We have N linear relations

$$K_s x_1 = x_s, \quad s = 0,2,3,\ldots,N. \tag{5.9}$$

With $\phi = 0$ we see that the conditions (3.24) become

$$K_s = s \pmod 2. \tag{5.10}$$

This is equivalent to the condition that the parity of the integers K_s coincides with the parity of s, that is, with the PST condition. We thus see that the PST condition is a special case of the APST condition, as expected.

A note is in order here. In general the translation $x_s \to x_s + \beta$ of the energy spectrum has no physical meaning: It is always possible to redefine the value of the ground-state energy and for instance to put it equal to zero as noted. (Similarly, the scale can be arbitrarily chosen using the dilation factor α.) This freedom relates to the values that the phase ϕ takes modulo 2π. For a given spectrum, the APST conditions might restrict ϕ; however, shifts in the ground-state energy will allow ϕ to take arbitrary values.

D. Spin chains with five sites and without magnetic field

Consider the the XX spin chain without magnetic fields ($B_0 = B_1 = \cdots = B_N = 0$) that contains five sites. In this case it is possible to express the APST conditions explicitly and to describe three possible scenarios: PST, APST, and neither.

This corresponds to $N = 4$. There are only two distinct exchange constants: J_1 and J_2. Indeed, due to the mirror-symmetry condition (3.23) we have (for $N = 4$) that $J_4 = J_1$, $J_3 = J_2$.

The spectrum of the corresponding Jacobi matrix J can easily be found:

$$x_0 = -a, \quad x_1 = -b, \quad x_2 = 0, \quad x_3 = b, \quad x_4 = a, \tag{5.11}$$

where $a = \sqrt{J_1^2 + 2J_2^2}$, $b = J_1$ are two positive parameters. Clearly, $a > b$ so the eigenvalues x_s in (5.11) are given in increasing order.

This is a special case of the situation considered in Sec. V A. The sufficient condition for APST is that the parameters a and b be linearly independent over the rationals. This is equivalent to the statement that the ratio a/b is an irrational number. We thus see that if $\sqrt{J_1^2 + 2J_2^2}/J_1$ is an irrational number, then the spin chain with five nodes has the APST property.

Suppose now that the ratio $a/b = n/m$ is a rational number where n,m are coprime integers. This means that there are two conditions on the eigenvalues

$$mx_0 - nx_1 = mx_4 - nx_3 = 0. \quad (5.12)$$

Then the relations (3.24) which are required for APST (with $\phi = 0$) reduce to the only condition that n be even and m be odd.

However, this is equivalent to the PST condition. Indeed, we have

$$\frac{a-b}{b} = \frac{n}{m} - 1 = M/m, \quad (5.13)$$

where M and m are both odd. Observe that the differences between the eigenvalues are $\Delta_1 = x_1 - x_0 = a - b$, $\Delta_2 = x_2 - x_1 = b$, $\Delta_3 = x_3 - x_2 = b$, $\Delta_4 = x_4 - x_3 = a - b$. Hence, Eq. (5.13) coincides with the PST condition for a chain with five sites.

In all other cases, that is, when n is odd and m is odd, or when both n and m are odd, the APST condition is not valid and the XX spin chain does demonstrate neither PST nor APST.

In the APST situation (i.e., when a/b is irrational), it is interesting to estimate the waiting times. It is easy to calculate the amplitude $f_{0N}(t)$ directly from

$$f_{0N}(t) = \frac{a^2 - b^2}{2a^2} + \frac{b^2}{2a^2}\cos at - \frac{1}{2}\cos bt. \quad (5.14)$$

This is a simple example of almost periodic functions: two harmonic oscillations with frequencies $\omega_1 = a$ and $\omega_2 = b$ do not constitute a pure periodic function. However, the Kronecker theorem guarantees that there exists a sequence t_n such that $f_{0N}(t_n) \to 1$ when $n \to \infty$.

There are several simple algorithms to estimate the quantities t_n.

One of them proceeds through the expansion of a/b into a continued fraction [20]

$$z = a/b = \zeta_0 + \frac{1}{\zeta_1 + \frac{1}{\zeta_2 + \cdots}}, \quad (5.15)$$

where the quotients $\zeta_0, \zeta_1, \ldots$ are integers. The corresponding convergents p_n/q_n of the continued fraction are rational numbers which provide the best approximation of the irrational number a/b [20]. In our case this method works well if all (or at least infinitely many) convergents have the property that p_n is even and q_n is odd. Otherwise, one can apply the method of Farey fractions [20] or, equivalently, the method of intermediate convergents [23].

This method can described as follows. Starting with the convergents $\{p_0/q_0, p_1/q_1, \ldots\}$ we compute the so-called mediants (or intermediate convergents) by the formula [23]

$$\frac{\tilde{p}_n}{\tilde{q}_n} = \frac{p_{n+1} \pm p_n}{q_{n+1} \pm q_n}. \quad (5.16)$$

The convergents p_n/q_n together with the intermediate convergents $\tilde{p}_n/\tilde{q}_n$ form a set of generalized convergents $w_n = u_n/v_n, n = 0,1,2,\ldots$, where $u_n = p_n$ or $u_n = \tilde{p}_n$ (similarly $v_n = q_n$ or $v_n = \tilde{q}_n$). From the elementary properties of the convergents it follows that all fractions u_n/v_n are simple (i.e., u_n and v_n are coprime). Moreover, it is possible to show [23] that the generalized convergents provide the general solution to the best approximation problem: They satisfy the inequality

$$|z - u_n/v_n| < v_n^{-2}. \quad (5.17)$$

It is easy to show that there are infinitely many generalized convergents u_n/v_n with the desired property: u_n is even while v_n is odd.

Indeed, assume that there is only a finite number of the convergents p_n/q_n with the desired property. This means that starting with some $n = M$ the numerators p_n are all odd; the corresponding denominators q_n may be either even or odd. Necessarily, for any neighbor pair p_n/q_n and p_{n+1}/q_{n+1}, the denominators q_n and q_{n+1} should be of opposite parity. Indeed, if one assumes that q_n and q_{n+1} have the same parity then their mediant $(p_n + p_{n+1})/(q_n + q_{n+1})$ will be reducible (with both numerator and denominator even), which is impossible. Thus, the mediants $\tilde{p}_n/\tilde{q}_n$ will have the desired property, because $\tilde{p}_n = p_{n+1} \pm p_n$ is even as a sum of two even numbers and $\tilde{q}_n = q_{n+1} \pm q_n$ is odd as a sum of two number with opposite parities. This means that for any irrational number $z = a/b$ there exists an infinite sequence of generalized convergents $c_n = u_n/v_n$ such that $\lim_{n\to\infty} c_n \to z$ and u_n is even while v_n is odd. Moreover, the best approximation property (5.17) holds for all such convergents.

Given this sequence, let us put

$$t_n = \frac{\pi v_n}{b}. \quad (5.18)$$

The amplitude $f_{0N}(t_n)$ then becomes

$$f_{0N}(t_n) = \frac{a^2 - b^2}{2a^2} + \frac{b^2}{2a^2}\cos\left(\pi v_n \frac{a}{b}\right) + \frac{1}{2}. \quad (5.19)$$

This can easily be simplified to

$$f_{0N}(t_n) = 1 - \frac{b^2}{a^2}\sin^2(\pi v_n \varepsilon_n/2), \quad (5.20)$$

where

$$\varepsilon_n = \frac{a}{b} - \frac{u_n}{v_n} \quad (5.21)$$

is the accuracy of the rational approximation of the irrational number a/b.

By property (5.17) we have that

$$f_{0N} \approx 1 - \frac{\pi^2 b^2}{a^2 v_n^2}. \quad (5.22)$$

It is seen from this formula that $f_{0N}(t_n)$ converges to 1 when $n \to \infty$. Moreover, this formula makes it possible to estimate the accuracy of this approximation if the (generalized) convergents u_n/v_n are known explicitly.

It is seen that $f_{0N}(t_n) \to 1$ when $t_n \to \infty$. This means that the sequence $\{t_n\}$ is associated with APST.

Consider the special case $J_1 = J_2 = 1$ so that all couplings are now equal. For the homogeneous Heisenberg chain (i.e., with $J_i = 1$ for all $i = 0,1,2,\ldots,N$) it is known [3] that PST only occurs when there are two or three sites. We are thus in a situation of APST for a uniform chain with five nodes.

In this case $a = \sqrt{3}$, $b = 1$. The continued fraction representation is

$$\sqrt{3} = 1 + \cfrac{1}{1 + \frac{1}{2 + \frac{1}{1+\cdots}}}. \tag{5.23}$$

The first convergents are

$$\frac{p_n}{q_n} = \left\{1,2,\frac{5}{3},\frac{7}{4},\frac{19}{11},\frac{26}{15},\frac{71}{41},\ldots\right\}. \tag{5.24}$$

It is seen that the first two convergents with the desired property (i.e., an even numerator and an odd denominator) are $2/1$ and $26/15$. Computing the mediants according to (5.16), we obtain the additional intermediate convergent $12/7$. Hence, the first three desired (intermediate) convergents are

$$\frac{u_n}{v_n} = \left\{\frac{2}{1},\frac{12}{7},\frac{26}{15}\right\}. \tag{5.25}$$

The first fraction, $2/1$, yields an approximation to the difference between $|f_{0N}(t)|$ and 1 with an accuracy of 3×10^{-1}; the second fraction $12/7$ yields an approximation with accuracy 2×10^{-2}.

So, already in the case of a spin chain with five sites we see that all three possibilities—PST, APST, or neither—can occur. APST is generic; that is, APST happens for almost all possible values of J_1 and J_2.

We consider next a XX spin chain with an *arbitrary* (even) number of spins which demonstrates the similar property.

E. Spin chain corresponding to the para-Krawtchouk polynomials

Assume that N is odd and that the spectrum x_s is such that (up to an affine transformation)

$$x_{2s} = 2s,\quad x_{2s+1} = 2s + \gamma,\quad s = 0,1,\ldots,(N-1)/2, \tag{5.26}$$

where γ is a real parameter such that $0 < \gamma < 2$.

This situation can be realized in spin chains that are obtained from the para-Krawtchouk polynomials with the recurrence coefficients [24]

$$B_n = \frac{\gamma + N - 1}{2},\qquad J_n^2 = \frac{n(N+1-n)[(N+1-2n)^2 - \gamma^2]}{4(N-2n)(N-2n+2)}. \tag{5.27}$$

The corresponding Jacobi matrix is mirror symmetric. When $\gamma = 1$ the grid is uniform and the Jacobi matrix J, which is associated to the ordinary Krawtchouk polynomials, generates PST [2].

It is clear that all eigenvalues can be expressed as linear combinations of x_1 and x_2. Indeed,

$$x_{2s} = s x_2,\quad x_{2s+1} = x_1 + s x_2,\quad s = 0,1,2,\ldots(N-1)/2. \tag{5.28}$$

Hence, according to our central result (3.24), in order to have APST, the following conditions must be realized:

$$a_{2s} = s a_2,\quad a_{2s+1} = a_1 + s a_2 \pmod{2\pi}, \tag{5.29}$$

where $a_s = \pi s - \phi$. These relations are compatible if and only if $\phi = 0 \pmod{2\pi}$.

If the parameter γ is irrational then there are no additional relations for the eigenvalues x_1, x_2 and thus provided (5.29) is verified, APST will occur.

Equivalently, this means that there exists a sequence $\{t_n, n = 1,2,\ldots\}$ such that

$$\lim_{n\to\infty} |f_{0N}(t_n)| = 1. \tag{5.30}$$

As in the previous case it is possible to determine the times t_n and estimate the corresponding rate of convergence in (5.30) using standard Diophantine approximation methods.

Indeed, we can always choose an infinite set of (intermediate) convergents $\{u_1/v_1, u_2/v_2, \ldots, u_n/v_n, \ldots\}$ with the property that the numerators u_n are all odd. Then we introduce the value

$$\varepsilon_n = \gamma - \frac{u_n}{v_n}, \tag{5.31}$$

which describes the accuracy of the Diophantine approximation of the parameter γ. We already saw that

$$|\varepsilon_n| < v_n^{-2}. \tag{5.32}$$

We choose

$$t_n = \pi v_n. \tag{5.33}$$

Substituting this in (3.14) and taking into account that u_n is odd we have

$$\begin{aligned} f_{0N}(t_n) &= -\sum_{s=0}^{(N-1)/2} w_{2s} + \sum_{s=0}^{(N-1)/2} e^{-i\pi\gamma v_n} w_{2s+1} \\ &= -\sum_{s=0}^{(N-1)/2} w_{2s} - e^{-i\pi v_n \varepsilon_n} \sum_{s=0}^{(N-1)/2} w_{2s+1}. \end{aligned} \tag{5.34}$$

In [24] it was shown that for the para-Krawtchouk polynomials the identities

$$\sum_{s=0}^{(N-1)/2} w_{2s} = \sum_{s=0}^{(N-1)/2} w_{2s+1} = 1/2 \tag{5.35}$$

hold. Hence,

$$f_{0N}(t_n) = -\tfrac{1}{2}(1 + e^{-i\pi v_n \varepsilon_n}). \tag{5.36}$$

Now

$$|f_{0N}(t_n)| = \cos(\pi v_n \varepsilon_n/2) \approx 1 - \frac{\pi^2}{8 v_n^2}, \tag{5.37}$$

where we have used Eq. (5.32).

Formula (5.37) gives a good approximation of the amplitude $|f_{0N}|$ if v_n is sufficiently large (depending on the physical requirements on the accuracy). For example, for $v_n > 10$ we get an accuracy of 1%.

Consider, for example, the value $\gamma = \sqrt{3}$.

From (5.23) we find the first appropriate (i.e., with all numerators u_n odd) convergents,

$$\frac{u_n}{v_n} = \left\{1,\frac{5}{3},\frac{7}{4},\frac{19}{11},\frac{45}{26},\frac{71}{41},\ldots,\right\}. \tag{5.38}$$

Already the third convergent $7/4$ gives an accuracy of about 1%. This is because the actual accuracy $\varepsilon_3 \approx 0.0179$ of the third convergent is smaller than the right-hand side of formula (5.32) gives. Hence, the first waiting time corresponding to an accuracy of 1% in the amplitude is $t_3 = 4\pi$.

Consider now the case where $\gamma = p/q$ is a rational number, with p and q coprime integers. In this case there is an additional linear relation between x_1 and x_2,

$$2qx_1 = px_2, \tag{5.39}$$

and hence a similar relation should hold for a_1 and a_2,

$$2qa_1 = pa_2 \pmod{2\pi}, \tag{5.40}$$

where $a_1 = \pi$, $a_2 = 2\pi$. If the numerator p is odd then (5.40) holds for any pair of coprime integers p,q and hence the APST condition is satisfied. In fact, we are then in the situation where not only APST but even PST occurs. Indeed, this corresponds to the model with PST that we derived and discussed in [24].

If the numerator $p = 2j$ is even for some integer j (in this case, necessarily the denominator q is odd) then relation (5.39) becomes $qx_1 = jx_2$ and hence (5.40) reads

$$q\pi - 2j\pi = 0 \pmod{2\pi}. \tag{5.41}$$

Obviously, (5.41) cannot hold when q is odd and there is no PST or APST in this case.

In summary, the picture is as follows:

(i) when γ is an irrational number, APST is observed;
(ii) when $\gamma = p/q$ is rational with p odd there is PST;
(iii) when $\gamma = p/q$ is rational with p even neither PST nor APST happens.

Let us make the following remark in connection with the last two examples. As mentioned in Sec. V C, in the discussion of the uniform XX chain, almost perfect return occurs in chains of the type we have been considering; this is so whenever the spectrum of the Jacobi matrix J is discrete. Clearly, this will be the case for any XX spin chain with nearest-neighbor interactions that has a finite number of sites. It should be stressed that finite length does not similarly imply APST; as we have seen, there are examples of systems with finite 1-excitation Hamiltonian J that do not possess APST.

VI. CONCLUSIONS

Let us recapitulate the essential elements of our analysis of APST in spin chains. It builds on the knowledge that XX spin chains with properly engineered couplings and magnetic fields can effect the transport of states from one end to the other with probability 1 over certain times; these are chains with PST. In view of the fact that there are always manufacturing or measurement imprecisions, our study aimed to characterize the models where although not perfect, state transfer could be realized with a probability very close to 1; such chains have been said to show APST.

We have thus undertaken to categorize all XX spin chains with arbitrary nearest-neighbor couplings and magnetic fields that would exhibit APST. The Kronecker theorem in Diophantine approximation proved essential in this investigation. The necessary and sufficient conditions that have been found for a chain to admit APST bear on the 1-excitation restriction J (a tridiagonal matrix) of the chain Hamiltonian. Not unlike what is needed for PST, the requirements for APST entail a symmetry condition on J as well as spectral restrictions. As it turns out, like for PST, J must be mirror-symmetric, that is, invariant against reflection with respect to its antidiagonal. The conditions on the eigenvalues of J turn out (in general) to be much less demanding for APST than for PST. They amount roughly to the conditions for which the Kronecker theorem applies and imply that at least a subset of these eigenvalues be linearly independent over the field of the rational numbers. Spin chains with APST therefore much enlarge, in principle, the class of such systems that can be exploited as quantum wires since their fidelity can be as good as is technically relevant.

It has also been demonstrated how chains with APST can be constructed from a chain that already admits (or possibly not) APST by the removal of single excitation energy levels from the parent system via Christoffel transforms. This offers a constructive method to broaden the catalog of systems with APST.

A number of examples and special cases interesting in their own right have also been presented and discussed. They illustrate situations where PST or APST occur or where neither can happen. One of the models introduced has provided counterexamples to the view borne out in particular from the examination of the Heisenberg XX chain with homogeneous couplings, that APST requires excessively long times in extended wires.

We trust this report provides interesting information on the transfer of state in XX spin chains with nearest-neighbor couplings and suggests that APST requires further analysis.

ACKNOWLEDGMENTS

A.Z. thanks Centre de Recherches Mathématiques (Université de Montréal) for hospitality. The authors would like to thank M. Christandl, M. Derevyagin, and A. Filippov for stimulating discussions. They also acknowledge communications from M. Bruderer, D. Burgarth, and S. Severini and are also very grateful to a referee for a very constructive and stimulating review. The research of LV is supported in part by a research grant from the Natural Sciences and Engineering Research Council (NSERC) of Canada.

[1] S. Bose, Contemp. Phys. **48**, 13 (2007).
[2] C. Albanese, M. Christandl, N. Datta, and A. Ekert, Phys. Rev. Lett. **93**, 230502 (2004).
[3] M. Christandl, N. Datta, Tony C. Dorlas, A. Ekert, A. Kay, and A. J. Landahl, Phys. Rev. A **71**, 032312 (2005).
[4] A. Kay, Phys. Rev. A **73**, 032306 (2006).
[5] R. Ronke, T. Spiller, and I. D'Amico, J. Phys.: Conf. Ser. **286**, 012020 (2011).
[6] D. Burgarth and S. Bose, Phys. Rev. A **71**, 052315 (2005).
[7] C. Marletto, A. Kay, and A. Ekert, Quantum Inf. Comput. **12**(7 & 8), 0648 (2012).
[8] G. De Chiara, D. Rossini, S. Montenegro, and R. Fazio, Phys. Rev. A **72**, 012323 (2005).
[9] C. K. Burrell and T. J. Osborne, Phys. Rev. Lett. **99**, 167201 (2007).

[10] C. K. Burrell, J. Eisert, and T. J. Osborne, Phys. Rev. A **80**, 052319 (2009).

[11] M. Bruderer, K. Franke, S. Ragg, W. Belzig, and D. Obreschkow, Phys. Rev. A **85**, 022312 (2012).

[12] A. Kay, Int. J. Quantum Inf. **8**, 641 (2010).

[13] L. Vinet and A. Zhedanov, Phys. Rev. A **85**, 012323 (2012).

[14] D. Burgarth, Ph.D. thesis, University College London, 2006.

[15] C. Godsil, Discrete Math. **312**, 129 (2012).

[16] C. Godsil, S. Kirkland, S. Severini, and J. Smith, Phys. Rev. Lett. **109**, 050502 (2012).

[17] A. Grünbaum, L. Vinet, and A. Zhedanov, arXiv:1205.4689.

[18] T. Chihara, *An Introduction to Orthogonal Polynomials* (Gordon and Breach, New York, 1978).

[19] A. S. Besicovitch, *Almost Periodic Functions* (Dover, Mineola, NY, 1954).

[20] G. H. Hardy and E. M. Wright, *An Introduction to the Theory of Numbers*, 6th ed. (Oxford University Press, Oxford, 2008).

[21] B. M. Levitan and V. V. Zhikov, *Almost Periodic Functions and Differential Equations* (Cambridge University Press, Cambridge, 1982).

[22] T. Shi, Y. Li, A. Song, and C. P. Sun, Phys. Rev. A **71**, 032309 (2005).

[23] S. Lang, *Introduction to Diophantine Approximations* (Springer-Verlag, Berlin, 1991).

[24] L. Vinet and A. Zhedanov, J. Phys. A: Mathematical and Theoretical **45**, 265304 (2012).