How to construct spin chains with perfect state transfer

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A method to systematically construct the XX quantum spin chains with nearest-neighbor interactions that allow perfect state transfer (PST) is shown. Sets of orthogonal polynomials (OPs) are in correspondence with such systems. The key observation is that for any admissible one-excitation energy spectrum, the weight function of the associated OPs is uniquely prescribed. This entails the complete characterization of these PST models with the mirror-symmetry property arising as a corollary. A simple and efficient algorithm to obtain the corresponding Hamiltonians is presented. A model connected to a special case of the symmetric q-Racah polynomials is offered. An explanation of how additional models with PST can be derived from a parent system by removing energy levels from the one-excitation spectrum of the latter is given. This is achieved through Christoffel transformations and is also completely constructive in regards to the Hamiltonians.

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I. INTRODUCTION

The problem of perfect state transfer (PST) in quantum information processing is deservedly attracting much attention. (See Refs. [1,2] for reviews.) The transport of the quantum state from one location to another is perfect if it is realized with probability 1, thereby avoiding dissipation. Occurrences of perfect transmission have been found in some XX chains with inhomogeneous couplings [1–4]: in these cases, the probability for the transfer of a single spin excitation from one end of the chain to the other is indeed found to be 1 for certain times. These models have the advantage that the perfect transfer can be done without the need for active control. We shall here describe how such systems can be systematically "constructed" from given one-excitation spectra.

Specifically, we shall focus on Hamiltonians H of the XX type with nearest-neighbor interactions, i.e.,

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

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 ($l = 0,1,\ldots,N$). The symbols σ_l^x, σ_l^y, and σ_l^z stand for the Pauli matrices, which act on the single-qubit states $|0\rangle$ and $|1\rangle$ as follows:

$$\sigma^x|0\rangle = |1\rangle, \quad \sigma^y|0\rangle = -i|1\rangle, \quad \sigma^z|0\rangle = -|0\rangle,$$
$$\sigma^x|1\rangle = |0\rangle, \quad \sigma^y|1\rangle = i|0\rangle, \quad \sigma^z|1\rangle = |1\rangle.$$

It is straightforward to see that

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

and therefore the eigenstates of H split in subspaces labeled by the number of spins over the chain that are in state $|1\rangle$. For our purposes, it will suffice to restrict H to the subspace spanned by the states which contain only one excitation (or spin up). A natural basis for that subspace is given by the vectors

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

where the only "1" occupies the nth position. In that basis, the restriction J of H to the one-excitation subspace is given by the following $(N+1)\times(N+1)$ Jacobi matrix:

$$J = \begin{pmatrix} B_0 & J_1 & 0 & & \\ J_1 & B_1 & J_2 & 0 & \\ 0 & J_2 & B_2 & J_3 & \\ & & \ddots & \ddots & \\ & & \cdots & J_N & B_N \end{pmatrix},$$

where it is assumed that $J_i > 0$. Its action on the basis vectors $|e_n)$ reads

$$J|e_n) = J_{n+1}|e_{n+1}) + B_n|e_n) + J_n|e_{n-1}). \tag{2}$$

Note also that the conditions

$$J_0 = J_{N+1} = 0 \tag{3}$$

are assumed.

It has been shown [2] that the eigenvalues of J must satisfy a simple PST condition for the perfect state transfer to be possible. (We shall discuss this in Sec. III.) Since they encode three-term recurrence relations, the Jacobi matrices are diagonalized by orthogonal polynomials (OPs). Spin chains allowing PST are hence in correspondence with families of OPs.

One question we address here is the following: Given spectral data sets satisfying the PST condition, can the corresponding spin chains with the PST property be found? In other words, is there a procedure to explicitly obtain the parameters J_n and B_n that determine the Hamiltonians? As it turns out, this question has a rather elegant, affirmative answer. Indeed, we shall see that the condition for a spin chain to possess the PST property is very simply expressed through the weight function of the orthogonal polynomials associated to the chain. Hence, given a set of eigenvalues satisfying the PST condition, the weight function is then prescribed. This uniquely fixes (up to normalization) the corresponding

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orthogonal polynomials and, therefore, the coefficients J_n and B_n as their recurrence coefficients. A simple algorithm for constructing spin chains with the PST property along these lines will be presented.

Another constructive issue that we consider is this: Can one obtain different spin chains with the PST property by performing some appropriate surgery on the spectrum of a model already known to generate PST? Here again the answer is positive and also provides tools to explicitly construct many spin chains with PST from a given one.

These two natural questions have been touched upon in [4,5]. However, the link with the weight function of the associated OPs have so far not been stressed, and therein lies the constructive power that our considerations add.

The outline of the paper is as follows.

In Sec. II, we briefly describe standard results concerning Jacobi matrices and orthogonal polynomials.

In Sec. III, we revisit the necessary and sufficient conditions for XX spin chains to realize perfect state transfer. We derive the spectral condition already referred to and obtain the expression for the weight function of the associated polynomials on which much of the model characterization hinges.

The approach fundamentally relies on the spectral theorem and therefore relates to many other circumstances (see, for example, [6,7]) where transition probabilities are likewise determined.

In Sec. IV, we offer a simple algorithm for constructing the Hamiltonians of the chains with PST from the spectra and the weight functions.

In Sec. V, we give two simple examples that illustrate how the proposed method applies. The first is the well-known case corresponding to a linear spectrum and the Krawtchouk polynomials. The second stems from a hyperbolic energy spectrum and leads to a spin chain Hamiltonian with PST that can be analytically described.

In Sec. VI, we present a "surgical" procedure consisting of the removal of energy levels from the one-excitation spectrum of a spin chain with PST. It is shown to lead to other spin chains with the same property. This spectral surgery amounts to performing Christoffel transforms of the orthogonal polynomials associated to the parent or original system. Since the transformed polynomials are explicitly known (from the general OP theory [8]), such is also the case for the corresponding Jacobi matrix and spin chain Hamiltonian.

II. FINITE JACOBI MATRICES AND ORTHOGONAL POLYNOMIALS

Because the matrix J is Hermitian, there exists an eigenbasis $|s\rangle$ such that

$$J|s\rangle = x_s|s\rangle, \quad s = 0,1,\ldots,N. \tag{4}$$

The eigenvalues x_s are all real and nondegenerate, i.e., $x_s \neq x_t$ if $s \neq t$.

Consider the expansion of the eigenbasis $|s\rangle$ in terms of the basis $|e_n)$,

$$|s\rangle = \sum_{n=0}^{N} W_{sn}|e_n). \tag{5}$$

From (4), it is seen that the expansion coefficients W_{sn} satisfy

$$J_{n+1}W_{s,n+1} + B_nW_{sn} + J_nW_{s,n-1} = x_sW_{sn}. \tag{6}$$

Hence we can present them in the form

$$W_{sn} = W_{s0}\chi_n(x_s), \tag{7}$$

where $\chi_n(x)$ are polynomials satisfying the recurrence relation

$$J_{n+1}\chi_{n+1}(x) + B_n\chi_n(x) + J_n\chi_{n-1}(x) = x\chi_n(x) \tag{8}$$

and the initial conditions

$$\chi_0 = 1, \quad \chi_{-1} = 0. \tag{9}$$

Both bases $|e_n)$ and $|s\rangle$ are orthonormal, i.e.,

$$(e_m|e_m) = \delta_{nm}, \quad \langle s'|s\rangle = \delta_{ss'}.$$

Therefore, the matrix W_{sn} is orthogonal,

$$\sum_{n=0}^{N} W_{sn}W_{s'n} = \delta_{ss'}, \tag{10}$$

and similarly

$$\sum_{s=0}^{N} W_{sn}W_{sm} = \delta_{nm}. \tag{11}$$

From (11), it follows that the polynomials $\chi_n(x)$ are orthonormal on the finite set of spectral points x_s,

$$\sum_{s=0}^{N} w_s\chi_n(x_s)\chi_m(x_s) = \delta_{nm}, \tag{12}$$

where

$$w_s = W_{s0}^2 \tag{13}$$

play the role of discrete weights for the polynomials $\chi_n(x)$.

Note that

$$\sum_{s=0} w_s = \sum_{s=0} W_{s0}^2 = 1, \tag{14}$$

which amounts to the standard normalization condition for the weights.

We thus have the expansions

$$|s\rangle = \sum_{n=0}^{N} \sqrt{w_s}\chi_n(x_s)|e_n), \tag{15}$$

and similarly

$$|e_n) = \sum_{s=0}^{N} \sqrt{w_s}\chi_n(x_s)|s\rangle. \tag{16}$$

In what follows, it will be convenient to work with monic orthogonal polynomials,

$$P_n(x) = J_1J_2,\ldots,J_n\ \chi_n(x) = x^n + O(x^{n-1}). \tag{17}$$

They satisfy the recurrence relation

$$P_{n+1}(x) + B_nP_n(x) + U_nP_{n-1}(x) = xP_n(x), \tag{18}$$

where $U_n = J_n^2 > 0$.

The polynomials $P_n(x)$ satisfy the orthogonality relation

$$\sum_{s=0}^{N} P_n(x_s)P_m(x_s)w_s = h_n\,\delta_{nm}, \tag{19}$$

where

$$h_n = U_1U_2,\ldots,U_n.$$

By starting from the initial conditions $P_0 = 1, P_{-1} = 0$, it is possible to reconstruct all monic polynomials $P_n(x), n = 1,2,\ldots,N$ uniquely. The polynomial $P_{N+1}(x)$ will be

$$P_{N+1}(x) = (x - x_0)(x - x_1),\ldots,(x - x_N). \tag{20}$$

From the standard theory of orthogonal polynomials [8], it follows that the discrete weights can be expressed as

$$w_s = \frac{h_N}{P_N(x_s)P'_{N+1}(x_s)}, \quad s = 0,1,\ldots,N. \tag{21}$$

In what follows, we shall take the eigenvalues x_s to be in increasing order, i.e., we shall assume that

$$x_0 < x_1 < x_2 < \cdots < x_N. \tag{22}$$

Such an ordering is always possible because, by assumption, all eigenvalues x_s of the Hermitian matrix J are real and simple.

One can then present the expression for $P'_{N+1}(x_s)$ in the form

$$\begin{aligned} P'_{N+1}(x_s) &= (x_s - x_0)(x_s - x_1)\cdots \\ &\quad \times (x_s - x_{s-1})(x_s - x_{s+1})\cdots(x_s - x_N) \\ &= (-1)^{N+s}|P'_{N+1}(x_s)|. \end{aligned} \tag{23}$$

III. NECESSARY AND SUFFICIENT CONDITIONS FOR PERFECT QUANTUM STATE TRANSFER

A perfect quantum state transfer is realized if for some fixed time $T > 0$, one has

$$e^{iTJ}|e_0) = e^{i\phi}|e_N), \tag{24}$$

where ϕ is a real number. In other words, the initial state $|e_0)$ evolves over time T into the state $|e_N)$ (up to an inessential phase factor $e^{i\phi}$).

Expanding the states $|e_0)$ and $|e_N)$ in terms of the eigenstates $|s\rangle$ with the help of formula (16), we find that condition (24) is equivalent to

$$\chi_N(x_s) = e^{-i\phi}e^{iTx_s}, \quad s = 0,1,\ldots,N. \tag{25}$$

Now, on the one hand, since the polynomial $\chi_N(x)$ is real, it follows from (25) that

$$\chi_N(x_s) = \pm 1. \tag{26}$$

On the other hand, the orthogonal polynomials $\chi_n(x)$ possess the interlacing property [8]. In particular, any zero of the polynomial $\chi_N(x)$ should lie between two neighboring zeros x_s of the polynomial $\chi_{N+1}(x)$. This is possible only if the values 1 and -1 alternate in (26), namely, if

$$\chi_N(x_s) = (-1)^{N+s}, \quad s = 0,1,\ldots,N, \tag{27}$$

where we took into account the ordering (22), formula (23), and the positivity of the weights w_s in formula (21).

From (25), it follows that (27) is equivalent to the condition

$$e^{-i\phi}e^{iTx_s} = e^{i\pi s}e^{i\phi+\pi(N+2G_s)}, \tag{28}$$

where G_s are arbitrary integers.

As a result, we have the following condition for the spacings between the successive levels:

$$x_{s+1} - x_s = \frac{\pi}{T}M_s, \tag{29}$$

where M_s may be arbitrary, positive, odd numbers.

We thus derived the necessary conditions, given by (29) and (27), for a spin chain to realize perfect state transfer.

It is easily seen that these conditions are also sufficient.

From (27), (21), and (23), it is observed that (27) is equivalent to the condition

$$w_s = \frac{\kappa_N}{|P'_{N+1}(x_s)|} > 0, \tag{30}$$

where the normalization constant κ_N (chosen from the condition $w_0 + w_1 + \cdots + w_N = 1$) is not essential for our considerations. This formula can also be found in [9], where it occurs in connection with the inverse spectral problem for persymmetric matrices. (See below.)

This means that only condition (29) is crucial: once the eigenvalues x_s satisfy (29), the weights $w_s > 0$ are then uniquely determined (up to a common factor) via (30) and (23). In turn, the spectral points x_s together with the weights w_s are known to determine the Hermitian Jacobi matrix J uniquely [8]. Hence, from the sole knowledge of the spectral points x_s [satisfying condition (29)], we can uniquely reconstruct the spin chain Hamiltonians with the desired properties.

IV. RECONSTRUCTION OF THE MATRIX J FROM SPECTRAL DATA

Consider now the matrix J^*, which is obtained from J by a reflection with respect to the main counterdiagonal, i.e.,

$$J^* = RJR, \tag{31}$$

where the matrix R (reflection matrix) is

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

The matrix J^* has the same structure as the matrix J (i.e., J^* is a Hermitian three-diagonal matrix),

$$J^* = \begin{pmatrix} B_0^* & J_1^* & 0 & & \\ J_1^* & B_1^* & J_2^* & 0 & \\ 0 & J_2^* & B_2^* & J_3^* & \\ & & \ddots & \ddots & \\ & & \ldots & J_N^* & B_N^* \end{pmatrix},$$

with the coefficients

$$B_n^* = B_{N-n}, \quad J_n^* = J_{N+1-n}. \tag{32}$$

Consider the corresponding monic orthogonal polynomials $P_n^*(x)$ satisfying the recurrence relation

$$P_{n+1}^*(x) + B_n^* P_n^*(x) + U_n^* P_{n-1}(x) = x P_n^*(x). \tag{33}$$

In view of (31), the matrix J^* has the same eigenvalues, i.e., $x_s, s = 0,1,\ldots,N$, as the matrix J.

Hence, the polynomials $P_n^*(x)$ are orthogonal on the same finite set of spectral points,

$$\sum_{s=0}^{N} P_n^*(x_s) P_m^*(x_s) w_s^* = h_n^* \delta_{nm}, \tag{34}$$

but with another set of weights w_s^*. There is a remarkable relation between the weights w_s and w_s^* [10–12]:

$$w_s w_s^* = \frac{h_N}{[P'_{N+1}(x_s)]^2}. \tag{35}$$

Now, if J is mirror symmetric, that is, $J^* = J$, we must have $w_s^* = w_s$, and in view of (35), both sets of weights are equal and given by (30). A Jacobi matrix J with mirror symmetry hence defines a spin chain with PST. Conversely, if the matrix J leads to a system with PST, the weights w_s of the associated OPs must be given by formula (30). From (35), it then follows that $w_s^* = w_s$. This, in turn, implies that $J^* = J$, or in other words, that J is mirror symmetric. Note that in the mathematical literature, the matrices with the property $J^* = J$ are called persymmetric [9,13].

In summary, (27) is equivalent to the condition that the matrix J is mirror symmetric or persymmetric.

The fact that (29) and the mirror symmetry of the matrix J are necessary and sufficient for perfect state transfer was shown in [2].

As a result, the exploration of systems with perfect state transfer proceeded customarily through the search for Jacobi matrices with mirror symmetry. We have just seen that this property follows automatically from the prescription (30). This observation considerably simplifies the problem of finding spin chains with PST, as their determination from the weight formula (30) avoids the necessity to check the mirror symmetry of J.

At this point, to complete the practical recipe for the construction of spin chains with PST, we only need to provide an efficient algorithm to determine the matrix J from the spectrum.

One such possible algorithm (to reconstruct persymmetric matrices from spectral data) was given in [9]. We here propose another one, which seems more efficient, especially in view of the "spectral surgery" procedure to be presented in the next section.

First, we notice that the polynomial $\chi_N(x)$ can be reconstructed from (27) by the ordinary Lagrange interpolation procedure [14].

Indeed, $\chi_N(x)$ has degree N and takes $N+1$ prescribed values ± 1 at $N+1$ prescribed distinct points $x_0, x_1, \ldots, x_N$.

It follows that

$$\chi_N(x) = \sum_{s=0}^{N} (-1)^{N+s} \mathcal{L}_s, \tag{36}$$

where $\mathcal{L}_s$ are the standard Lagrange polynomials,

$$\mathcal{L}_s = \prod_{i=0}^{N\ \prime} \frac{x - x_i}{x_s - x_i} \tag{37}$$

[as usual, the symbol $'$ means that $i \neq s$ in the product (37)]. The monic polynomial $P_N(x)$ is then obtained through the division of $\chi_N(x)$ by the coefficient of its leading monomial.

We thus know explicitly two monic polynomials: $P_N(x)$ and $P_{N+1}(x) = (x - x_0)(x - x_1), \ldots, (x - x_N)$. Starting from these polynomials, it is possible to reconstruct, step by step, all of the orthogonal monic polynomials $P_n(x)$, $n = N-1, N-2, \ldots, 1$ by the well-known Euclidean algorithm.

Let us divide the polynomial $P_{N+1}(x)$ by the polynomial $P_N(x)$:

$$P_{N+1}(x) = q_N(x) P_N(x) + R_{N-1}(x), \tag{38}$$

where $q_n(x) = x - \beta_N$ and $R_{N-1}(x)$ is the residue of this division. By construction, we have, on the one hand, $\deg[R_{N-1}(x)] = N - 1$, and hence

$$R_{N-1}(x) = \gamma_N Q_{N-1}(x), \tag{39}$$

where $Q_{N-1}(x) = x^{N-1} + O(x^{N-2})$ is a monic polynomial of degree $N-1$.

On the other hand, we have the recurrence relation (18) from which we conclude that $\beta_N = b_N$, $\gamma_N = u_N$, and $Q_{N-1}(x) = P_{N-1}(x)$. We thus get the next monic orthogonal polynomial $P_{N-1}(x)$ as well as the recurrence coefficients b_N, u_N.

The same steps can then be repeated with the polynomials $P_N(x), P_{N-1}(x)$, yielding the recurrence coefficients b_{N-1}, u_{N-1} and the polynomial $P_{N-2}(x)$. Iteration will provide all recurrence coefficients, b_n, $n = 0,1,\ldots,N$ and u_n, $n = 1,2,\ldots,N$, together with the corresponding orthogonal polynomials, $P_n(x)$, $n = 1,2,\ldots,N$.

From a physical point of view, the case $B_n = 0$ is of special interest because it corresponds to zero external magnetic field. Jacobi matrices J with zero diagonal entries $B_n = 0$ correspond to symmetric orthogonal polynomials satisfying the property [8]

$$P_n(-x) = (-1)^n P_n(x). \tag{40}$$

Conversely, (40) is equivalent to the condition $B_n = 0$ in the Jacobi matrix J [8].

What is more important is that (40) is tantamount to the following spectral properties [8]:

(i) the eigenvalues are antisymmetric, i.e.,

$$x_n = -x_{N-n}, \quad n = 0,1,\ldots,N, \tag{41}$$

and

(ii) the weights are symmetric,

$$w_s = w_{N-s} > 0. \tag{42}$$

We can now apply these observations to the PST problem. Assume that the eigenvalues x_s satisfy the properties (29) and (41). Then, the weights w_s constructed from formula (30) obviously satisfy (42).

For perfect state transfer to be achieved in spin chains with zero magnetic field, it is thus necessary and sufficient that the one-excitation energies satisfy (29) and (41). A similar

result was obtained in [2] using a method associated to the inverse eigenvalue problem. Note that it is assumed in [2] that the matrix J is mirror symmetric. We already observed that this assumption is superfluous, as the mirror symmetry of J follows from (30).

V. TWO EXPLICIT EXAMPLES

As illustrations of how the constructive procedure we have described can be applied, we present in this section two examples.

Before proceeding, note that given a spectral data set x_s, $s = 0,1,\ldots,N$, it is straightforward to obtain another set satisfying (29) by an affine transformation,

$$\tilde{x}_s = \alpha x_s + \beta, \tag{43}$$

where α,β are arbitrary real parameters. The corresponding Jacobi matrix will then have, for its entries,

$$\tilde{B}_n = \alpha B_n + \beta, \quad \tilde{J}_n = \alpha J_n. \tag{44}$$

We can use this freedom to choose the most convenient form of the spectral data.

In particular, it is always possible to choose the parameters α,β so that the eigenvalues $\tilde{x}_s$ are integers with alternating parity (all x_{2s} even and all x_{2s+1} odd). We will use this observation in the following.

Consider first the uniform grid

$$x_s = s - N/2, \quad s = 0,1,\ldots N. \tag{45}$$

Using (30), we easily reconstruct the weights w_s to obtain the binomial distribution. The corresponding orthogonal polynomials $P_n(x;N)$ are the symmetric Krawtchouk polynomials, and the entries of the matrix J are

$$B_n = 0, \quad J_n^2 = \frac{n(N+1-n)}{4}. \tag{46}$$

This example is well known and was, in fact, obtained in [3] as an example of inhomogeneous spin chain with the perfect state transfer property.

Let us note that this system had also appeared much earlier in related contexts of coupling strength design. In [6], for instance, it was used to describe the excitation dynamics of an N-level problem; while in [7], it was employed to provide quantum computer models for which the result of a calculation is found for some prescribed time, at a given position, with probability 1.

The next example is less trivial and seems to have escaped notice. Take a "hyperbolic" analog of the uniform spectrum, i.e.,

$$x_s = A(q^{-s+N/2} - q^{-N/2+s}), \quad s = 0,1,\ldots,N, \tag{47}$$

where $0 < q < 1$ and A are real parameters. These parameters should be chosen so as to enforce the condition that all differences $x_{s+1} - x_s$ are positive odd integers. To that end, it is sufficient to demand that all x_s be integers with alternating parity: say x_0 is even, x_1 odd, x_2 even, and so on.

To do this, let us notice that the spectral points given by (47) satisfy the recurrence relation

$$x_{s+1} + x_{s-1} = (q + q^{-1})x_s, \quad s = 1,2,\ldots,N-1. \tag{48}$$

In order to ensure that all x_s are integers with alternating parity, we need to require

$$q + q^{-1} = K, \tag{49}$$

where $K = 4,6,\ldots$ is an arbitrary, positive, even integer in the case of even N, and $K = 6,10,14,18,\ldots$ in the case of odd N [we avoid the case $K = 2$ because it leads to the degenerate case $q = 1$ corresponding to the uniform grid (45)]. Condition (49) means that q is a special case of quadratic irrationality. The difference in the ranges of K for even N and odd N is explained by the observation that for even N, the minimal distance between the eigenvalues x_s is $A(q^{-1} - q)$, while for odd N, the minimal distance is $2A(q^{-1/2} - q^{1/2})$. The admissible values for K then easily follow from (48).

With the help of (30), the weights are straightforwardly found (up to a normalization factor):

$$w_s = (-1)^s\, q^{sN}(1 + q^{2s-N})\, \frac{(q^{-N};q)_s(-q^{-N};q)_s}{(q;q)_s(-q;q)_s}, \tag{50}$$

where

$$(x;q)_n = (1-x)(1-xq)\cdots(1-xq^{n-1})$$

stands for the q-shifted factorial [15].

The weights given by (50) correspond to a special case of the q-Racah polynomials that are orthogonal on the grid (47) [15]. Hence, the entries B_n, J_n of the Jacobi matrix J can be recovered from the known recurrence coefficients of the q-Racah polynomials [15].

The spectrum x_s is antisymmetric, $x_{N-s} = -x_s$, hence the diagonal terms are absent, i.e., $B_n = 0$. For the nondiagonal terms, we have, from [15], the expression

$$U_n = J_n^2 = A^2\, \frac{(1-q^{2n})(q^{2(n-N-1)} - 1)}{(1+q^{2n-N-2})(1+q^{2n-N})}. \tag{51}$$

It is easily seen that the coefficients (51) are positive and satisfy the mirror-symmetry condition $U_n = U_{N+1-n}$.

Another explicit example of PST spin chain related to the q-Krawtchouk polynomials was presented in [16].

VI. SPECTRAL SURGERY AND GENERATING NEW PST CHAINS

Given a one-excitation spectrum x_s, $s = 0,1,\ldots,N$ satisfying condition (29), we have seen how to construct the spin chain Hamiltonian with PST. The Jacobi matrix, which has the couplings and magnetic field strengths as its entries, is recovered from the prescribed weights w_s given by (30), or, in an equivalent form,

$$w_s = \frac{(-1)^{N+s}}{\prod_{i=0}^{N}{}'(x_s - x_i)}, \tag{52}$$

where it is assumed that $x_0 < x_1 < \cdots < x_N$. By construction, all weights are positive, i.e., $w_s > 0$, $s = 0,1,\ldots,N$. The weights w_s in (52) are defined up to an arbitrary positive common factor, which has no effect on the entries J_i, B_i of the Jacobi matrix J.

Consider the modified set of spectral data $x_1, x_2, \ldots, x_N$ obtained by removing the first entry x_0. The corresponding

weights,

$$\tilde{w}_s = \frac{(-1)^{N+s}}{\prod_{i=1}^{N}{}' (x_s - x_i)}, \quad s = 1,2,\ldots,N,$$

can be obtained from the initial weights in the following simple manner:

$$\tilde{w}_s = \text{const} \times (x_s - x_0) w_s. \tag{53}$$

This procedure removes the eigenvalue x_0 and preserves the positivity of the resulting weights w_s.

Similarly, one can remove any fixed spectral point x_j:

$$\tilde{w}_s = \text{const} \times (x_s - x_j) w_s, \quad s = 0,1,\ldots,j-1, \quad j+1,\ldots,N. \tag{54}$$

In this case, however, the new weights will be positive only if either $j = 0$ or $j = N$. In all other cases, the weights w_s cannot be positive for all s.

Nevertheless, removing a pair of neighboring points x_j, x_{j+1} through

$$\tilde{w}_s = \text{const} \times (x_s - x_j)(x_s - x_{j+1}) w_s \tag{55}$$

maintains positivity of the weights $\tilde{w}_s$ for all s, preserves property (29), and thus provides a new admissible Jacobi matrix $\tilde{J}$, which also generates perfect state transfer.

This procedure of removing pairs of neighboring levels can obviously be iterated.

The orthogonal polynomials $\tilde{P}_n(x)$ corresponding to the weights given by (54) are obtained from the polynomials $P_n(x)$ by the Christoffel transform [17],

$$\tilde{P}_n(x) = \frac{P_{n+1}(x) - A_n P_n(x)}{x - x_j}, \tag{56}$$

where

$$A_n = \frac{P_{n+1}(x_j)}{P_n(x_j)}.$$

The entries of the matrix $\tilde{J}$ are related to the entries of the matrix J by the well-known formulas [18]

$$\tilde{U}_n = U_n \frac{A_n}{A_{n-1}}, \quad \tilde{B}_n = B_{n+1} + A_{n+1} - A_n. \tag{57}$$

Formulas (56) and (57) can be applied iteratively in order to obtain new matrices $\tilde{J}$ with perfect state transfer from a matrix J with that property.

Assume now that the initial matrix J describes a dynamics with zero magnetic field, i.e., $B_n = 0$. The spectral points x_s satisfy, therefore, the symmetry condition (41). In this case, one may remove a symmetric pair of boundary eigenvalues corresponding to the first and last levels,

$$\tilde{w}_s = \text{const} \times \left(x_s^2 - x_0^2\right) w_s, \tag{58}$$

and find, for the associated polynomials $\tilde{P}_n(x)$ [17],

$$\tilde{P}_n(x) = \frac{P_{n+2}(x) - K_n P_n(x)}{x^2 - x_0^2}, \quad K_n = \frac{P_{n+2}(x_0)}{P_n(x_0)}, \tag{59}$$

therefore obtaining a new Jacobi matrix $\tilde{J}$ with zero magnetic field $\tilde{B}_n = 0$ and with

$$\tilde{U}_n = U_n \frac{K_n}{K_{n-1}}. \tag{60}$$

If N is odd, there is another possibility to remove two neighboring levels, in this case from the middle of the spectrum. Indeed, take

$$\tilde{w}_s = \text{const} \times (x_s - x_j)(x_s - x_{j+1}) w_s = \text{const} \times \left(x_s^2 - x_j^2\right) w_s, \tag{61}$$

where $j = (N-1)/2$. Formulas (59) and (60) remain valid if one replaces x_0 with x_j.

The idea of obtaining PST chains with $B_n = 0$ from given ones was discussed in [5]. Our approach is much more explicit and exploits well-known formulas from the theory of orthogonal polynomials.

As a simple (but already nontrivial) example, consider the removal of levels from the middle of the uniform spectrum (45) with odd N. After a finite number L of such transformations, we obtain spectral data of the form

$$x_s = -N/2, -N/2+1, \ldots, -L-3/2, -L-1/2, L+1/2, L+3/2, \ldots, N/2-1, N/2. \tag{62}$$

For $L = 0$, this spectral data set coincides with (45). For $L = 1,2,\cdots < (N-1)/2$, we have two uniform grids separated by a gap of length $2L+1$. This spectrum corresponds to a spin chain with $B_n = 0$ that has the perfect transfer of state property, and that was introduced in [19] and studied in [20]. We have shown in [21] that this model is associated to the dual -1 Hahn polynomials.

Let us conclude by stressing here that *all* spin chains with the PST property (not only those with $B_n = 0$ as in [5]) can be obtained through such (iterated) spectral surgery from the PST spin chain corresponding to the uniform grid (45).

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