Analytic next-to-nearest-neighbor *XX* models with perfect state transfer and fractional revival

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Certain nonuniformly coupled spin chains can exhibit perfect transfer of quantum states from end to end. Motivated by recent experimental implementations in evanescently coupled waveguide arrays, we extend the simplest such chain to next-to-nearest-neighbor couplings. It is shown analytically that perfect state transfer can be maintained under the extension and that end-to-end entanglement generation (fractional revival) can occur.

I. INTRODUCTION

A. Background

The transfer of quantum states between remote sites is an important issue in the development of quantum technologies. Theoretical studies have shown that over short distances spin chains could achieve this task with a minimum of control operations (see Ref. [1] and the recent review Ref. [2]). Indeed, with properly engineered couplings, the intrinsic dynamics of the chain can realize the transfer with unit probability, in which case one speaks of perfect state transfer (PST) [3–5]. Another phenomenon, known as fractional revival (FR) [6], can also be observed in spin chains [4,7–11] and exploited for quantum communication purposes. In this case, an excitation on one end of the chain splits into a superposition of an excitation at each end, resulting in entanglement between the ends of the chain.

The class of spin chain Hamiltonians that has been principally examined in this connection is that of type *XX* with nearest-neighbor (NN) couplings,

$$H = \frac{1}{2}\sum_{n=0}^{N-1} J_l\big(\sigma_n^x\sigma_{l+1}^x + \sigma_n^y\sigma_{n+1}^y\big) + \frac{1}{2}\sum_{n=0}^{N} B_n\big(\sigma_n^z + 1\big), \quad (1)$$

where the $\sigma_l^{x/y/z}$ denote the corresponding Pauli matrix acting on site l. Owing to rotational symmetry about one axis, the total spin projection is conserved in these models and the space of states decomposes into a sum of subspaces labeled by the number of excitations. PST is then determined by the one-excitation dynamics. Restricting to this dynamics, H takes the form of a tridiagonal matrix given by

$$\begin{pmatrix} B_0 & J_1 & & & \\ J_1 & B_1 & J_2 & & \\ & J_2 & B_2 & \ddots & \\ & & \ddots & \ddots & J_N \\ & & & J_N & B_N \end{pmatrix}. \quad (2)$$

Families of orthogonal polynomials that have the matrix entries as their recurrence coefficients provide the exact eigenfunctions. Consequently, the correspondence between orthogonal polynomials has been investigated and many chains with PST have been found using this correspondence [5,12–14]. The simplest and thus paradigmatic model in this context is associated to the Krawtchouk polynomials. The couplings

in this case follow an elementary parabolic distribution,

$$J_n = a_n \equiv \frac{1}{2}\sqrt{n(N-n+1)}, \quad (3)$$

and there are no Zeeman terms, $B_n = 0$. The Krawtchouk chain does not exhibit fractional revival, but models that do have been found and indeed been analyzed systematically [10,11,15].

B. Recent experiments

Perfect state transfer has been demonstrated recently in different technological platforms. Perfect state transfer and the stronger mirror inversion have been observed using nuclear magnetic resonance techniques [16]. Since the time evolution of a single excitation is mathematically equivalent to an excitation in a lattice of oscillators in the tight binding formalism with nearest-neighbor approximation (only when multimodes are considered differences between fermions and bosons appear), photonic lattice implementations of perfect state transfer have been considered [17–20]. Indeed, it has been demonstrated experimentally that quantum states can be transported with high fidelity through arrays of evanescently coupled waveguide elements [21–23]. The present paper is largely motivated by these advances. Since the evanescent couplings of the wave guides in an optical array depend on the separation between the components, interactions always extend beyond the nearest neighbors and a better approximate description would involve next-to-nearest couplings. It could also be that manufacturing or setting imprecisions would have the array in a slight zigzag pattern in which case the NNN couplings can become even more significant relative to the NN couplings [24]. The same could happen, of course, if the quantum network is bent [25].

These considerations call for an examination of PST in models with NNN interactions in addition to the NN ones. Such a study would provide a framework to better estimate the errors made when the NNN couplings are neglected, it could inform the situations when these couplings are really required and, finally, it could unveil new dynamical possibilities when NNN interactions are present. The question of PST beyond NN couplings has been addressed in Ref. [26], where it has been shown that inverse spectral problem methods can be applied to obtain Hamiltonians with interactions beyond the nearest neighbors that exhibit PST. See also Ref. [27] in this connection. This work, however, is numerical and, to our knowledge, no such analytic models have been identified so far.

C. Our contribution

The purpose of this paper is precisely to fill that lacuna and to offer a simple analytic model with PST and also FR that naturally extends the Krawtchouk model. The nearest-neighbor couplings $J_n^{(1)}$ of this model remain the same as those of the Krawtchouk XX spin chains with a scaling factor β,

$$J_n^{(1)} = J_n = \beta a_n,$$

the next-to-nearest neighbor couplings $J_n^{(2)}$ involve an additional parameter α and nonuniform magnetic fields are present:

$$J_n^{(2)} = \alpha a_{n-1} a_n, \quad B_n = \alpha\left(a_n^2 + a_{n+1}^2\right). \tag{4}$$

PST will be shown to happen when $\frac{\alpha}{\beta}$ is rational. For some of these values, it might be necessary to have an odd or even number of sites. If $\frac{\alpha}{\beta}$ is an integer, it will be seen that the minimal time for PST in the NNN chains is the same as the one with the NN couplings.

It will further be seen that, in many instances, the model with the NNN couplings will exhibit FR. This is in contrast with the fact that this phenomenon does not take place in the Krawtchouk chain with only nearest-neighbor couplings.

D. Paper structure

The paper is structured as follows. In Sec. II we introduce the basics of the nonuniform XX chain and review in more detail mirror symmetry in the nearest-neighbor situation. We also introduce the special class of next-to-nearest-neighbor chains we will consider in this paper. In Sec. III, we study general conditions for perfect state transfer in XX chains and discuss in detail the well-known Krawtchouk case for nearest-neighbor couplings. We then characterize as one main result of this study perfect state transfer in the next-to-nearest-neighbor extension of the Krawtchouk case. In Sec. IV we turn our attention to fractional revival and give also here an exact characterization of our Krawtchouk extension. In Sec. V we offer a conclusion and an outlook.

II. PRELIMINARIES

A. Spin chains of XX type

Consider the following Hamiltonians of type XX on $(\mathbb{C}^2)^{\otimes(N+1)}$ where each of the $(N+1)$ spins interacts with its M neighbors on the left and M neighbors on the right:

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

$$+ \frac{1}{2} \sum_{l=0}^{N} B_l\left(\sigma_l^z + 1\right).$$

The constant $J_{l+k}^{(k)}$ is the coupling strength between the site l and $l+k$ and is taken to be nonnegative; the constant B_l is the value of the magnetic field at the site l.

Since, the z component of the total spin is conserved,

$$\left[H^{(M)}, \frac{1}{2} \sum_{l=0}^{N}\left(\sigma_l^z + 1\right)\right] = 0, \tag{5}$$

the eigenstates of $H^{(M)}$ belong to subspaces labeled by the number of spins over the chain that are up, i.e., that are eigenstates of σ^z with eigenvalue $+1$. The state of $H^{(M)}$ with all the spins down has energy zero. It will suffice for our purposes to consider states with only one spin up (for a detailed explanation of this point, see Ref. [4]). A natural basis for that subspace (equivalent to $\mathbb{C}^{(N+1)}$) is given by the vectors

$$|n\rangle = (0,0,\ldots,1,\ldots,0)^T \tag{6}$$

$n = 0, \ldots, N$, with the only 1 in the nth position corresponding to the only spin up at the nth site. The action of $H^{(M)}$ on those states is given by

$$H^{(M)}|n\rangle = J_{n+M}^{(M)}|n+M\rangle + J_{n+M-1}^{(M-1)}|n+M-1\rangle + \ldots$$

$$+ J_{n+1}^{(1)}|n+1\rangle + B_n|n\rangle + J_n^{(1)}|n-1\rangle$$

$$+ \cdots + J_n^{(M)}|n-M\rangle. \tag{7}$$

The conditions $J_l^{(k)} = 0$ for $l \leqslant k-1$ and $J_{N+1}^{(k)} = 0$ are assumed.

In the following we shall consider models whose non-nearest-neighbor couplings are constructed from the interaction strengths between the nearest neighbors. At one point, we shall spell out a model with $M = 2$, but the way for extending to arbitrary M will be clear in principle. We shall hence make much use of the description of the single excitation dynamics when only nearest neighbors are coupled; its essentials are summarized in the next subsection.

B. Nearest-neighbor interactions

This subsection offers background on the relevant elements of orthogonal polynomial theory and establishes some notation.

When $M = 1$, there are only nearest-neighbor interactions. Let us denote by J the restriction of $H^{(1)}$ to the single-excitation eigensubspace. It is readily seen that Eq. (7) specializes to

$$H^{(1)}|n\rangle \equiv J|n\rangle = J_{n+1}|n+1\rangle + B_n|n\rangle + J_n|n-1\rangle, \tag{8}$$

where we have replaced $J_n^{(1)}$ by J_n for simplicity. We thus see that in the occupation basis, J can be represented by the $(N+1) \times (N+1)$ tridiagonal matrix Eq. (2) given above.

Introduce the normalized eigenvectors $|x_s\rangle$ of J:

$$J|x_s\rangle = x_s|x_s\rangle, \quad s = 0,1,\ldots,N. \tag{9}$$

The eigenvalues x_s are real and nondegenerate: $x_s \neq x_t$ if $s \neq t$, for positive couplings. Let us expand the eigenstates $|x_s\rangle$ in terms of the basis vectors $|n\rangle$:

$$|x_s\rangle = \sum_{n=0}^{N} W_{sn}|n\rangle, \tag{10}$$

and write the expansion coefficients as follows:

$$W_{sn} = W_{s0}\chi_n(x_s), \tag{11}$$

with $\chi_0(x_s) = 1$ by construction. Set $\sqrt{w_s} = W_{s0}$. Relation Eq. (10) becomes

$$|x_s\rangle = \sum_{n=0}^{N} \sqrt{w_s} \chi_n(x_s)|n\rangle. \qquad (12)$$

It follows from Eq. (8) that the coefficients $\chi_n(x)$ obey the three-term recurrence relation

$$J_{n+1}\chi_{n+1}(x) + B_n\chi_n(x) + J_n\chi_{n-1}(x) = x\chi_n(x) \qquad (13)$$

and are hence orthogonal polynomials with the initial condition $\chi_{-1} = 0$ added. Since the eigenbasis and the occupation basis are both orthonormal and given that the expansion coefficients are real, these elements form an orthogonal matrix and provide the inverse relations

$$|n\rangle = \sum_{s=0}^{N} \sqrt{w_s} \chi_n(x_s)|x_s\rangle. \qquad (14)$$

Now the fact that $\langle n|m\rangle = \delta_{nm}$ implies that

$$\sum_{s=0}^{N} w_s \chi_n(x_s)\chi_m(x_s) = \delta_{nm}, \qquad (15)$$

showing that the polynomials $\chi_n(x)$ are orthogonal over the finite set of eigenvalues x_s of J with weight w_s. From the eigenvalues x_s, $s = 0, 1, \ldots, N$ one can form the characteristic polynomial $P_{N+1}(x)$ of degree $N + 1$:

$$P_{N+1}(x) = (x - x_0)(x - x_1) \ldots (x - x_N), \qquad (16)$$

which is obviously orthogonal to all $\chi_n(x)$ $n = 0, 1, \ldots, N$ according to Eq. (15). It is known from the theory of orthogonal polynomials [28] that the discrete weights w_s can be expressed as

$$w_s = \frac{\sqrt{h_N}}{\chi_N(x_s)P'_{N+1}(x_s)} \quad s = 0, 1, \ldots, N, \qquad (17)$$

where

$$\sqrt{h_N} = J_1 J_2 \ldots J_N \qquad (18)$$

and where $P'_{N+1}(x)$ stands for the derivative of $P_{N+1}(x)$. If one takes the eigenvalues in increasing order,

$$x_0 < x_1 < \cdots < x_N, \qquad (19)$$

it is easy to see that

$$P'_{N+1}(x_s) = (-1)^{N+s}|P'_{N+1}(x_s)|. \qquad (20)$$

The class of mirror-symmetric couplings and field strengths satisfying

$$J_n = J_{N+1-n}, \quad B_n = B_{N-n} \qquad (21)$$

is central in PST considerations (see, for instance, Refs. [4,5,12]). In terms of the matrix J given in Eq. (2), the conditions Eq. (21) amount to the requirement that J be reflection invariant with respect to its main antidiagonal and thus satisfy $RJ = JR$ with

$$R = \begin{pmatrix} 0 & \ldots & 0 & 1 \\ 0 & \ldots & 1 & 0 \\ & \ddots & & \\ 1 & 0 & \ldots & 0 \end{pmatrix} \qquad (22)$$

the matrix transcription of the reflection defined by $R|n\rangle = |N - n\rangle$. Observe that $R^2 = 1$. When J and R commute, they can be diagonalized simultaneously and since the eigenstates $|x_s\rangle$ are nondegenerate, we have then

$$R|x_s\rangle = \epsilon_s|x_s\rangle, \qquad (23)$$

with $\epsilon_s = \pm 1$. Moreover, from Eq. (12) we obtain

$$R|x_s\rangle = \sum_{n=0}^{N} \sqrt{w_s} \chi_n(x_s)|N - n\rangle$$

$$= \sum_{n=0}^{N} \sqrt{w_s} \chi_{N-n}(x_s)|n\rangle. \qquad (24)$$

Equations (23) and (24) thus yield

$$\chi_{N-n}(x_s) = \epsilon_s \chi_n(x_s). \qquad (25)$$

It can also be shown [12] that in the presence of mirror symmetry the weights are given by

$$w_s = \frac{\sqrt{h_N}}{|P'_{N+1}(x_s)|}. \qquad (26)$$

Comparing Eq. (26) with the general formula Eq. (15) and using Eq. (20) allows us to show that

$$\chi_N(x_s) = (-1)^{N+s} \qquad (27)$$

is equivalent to the condition that the matrix J be mirror-symmetric. Setting $n = 0$ in Eq. (25), one further concludes that

$$\epsilon_s = (-1)^{N+s} \qquad (28)$$

and then obtains from Eq. (25) the following property of orthogonal polynomials associated to mirror-symmetric Jacobi matrices:

$$\chi_{N-n}(x_s) = (-1)^{N+s} \chi_n(x_s). \qquad (29)$$

C. From nearest-neighbor to non-nearest-neighbor couplings

As seen from Eq. (7), the couplings and magnetic field strengths of the Hamiltonians $H^{(M)}$ are in fact determined from the restriction of $H^{(M)}$ to the one-excitation subspace. In the following, we shall consider a special class of $H^{(M)}$ where the non-nearest-neighbor couplings are prescribed from those between the nearest neighbors. We shall define these special Hamiltonians by demanding that their restriction to states with only one spin up takes the form

$$H^{(M)}|n\rangle = Q_M(\bar{J})|n\rangle, \qquad (30)$$

where Q_M is a polynomial of degree $M < N$ in a fiducial tridiagonal matrix $\bar{J}$ of the same form as Eq. (2) with entries that can be viewed as basic nearest-neighbor couplings and field strengths. From the action of $\bar{J}$ on $|n\rangle$ given by Eq. (8) with J_n and B_n replaced by $\bar{J}_n$ and $\bar{B}_n$, respectively, it is straightforward to compute $Q_M(\bar{J})|n\rangle$ and to identify the couplings $J_l^{(k)}$ of $H^{(M)}$ (see Sec. III D for an explicit example in the case $M = 2$).

This will provide families of Hamiltonians where the spin at site n interacts with its M neighbors on the left and on the right; we shall henceforth limit our considerations to this special

class of systems with non-nearest-neighbor interactions. Note that the multiexcitation states of spin chains with interactions beyond nearest neighbors, such as those considered here, will not be mapped onto free fermion states by the Jordan-Wigner transformation.

The formalism developed above applies generally to tridiagonal matrices and hence to $\bar{J}$. In the following, we shall wish to distinguish between $\bar{J}$ and $J^{(1)} = J$. Typically, we shall have $J = \beta \bar{J}$ with β a constant determined by experimental parameters. For clarity, when using the results of Sec. II as they pertain to $\bar{J}$, we shall denote by $\bar{x}_s$ the eigenvalues of $\bar{J}$, by $\bar{\chi}_n$ the orthonormalized polynomials associated to $\bar{J}$, etc.

III. PERFECT STATE TRANSFER

A. General considerations

Let us now explore the conditions for the transfer with probability one, after time T, of a spin up from one end of the chain to the other, when the dynamics is governed by the special Hamiltonians $H^{(M)}$ defined by Eq. (30). This PST will be realized if

$$e^{-iTH^{(M)}}|0\rangle = e^{i\phi}|N\rangle, \qquad (31)$$

where ϕ is some phase. With the help of the expansion Eq. (14) and with a bar over the attributes of $\bar{J}$, we see that condition Eq. (31) amounts to

$$e^{-i\phi} \exp[-iT Q_M(\bar{x}_s)] = \bar{\chi}_N(\bar{x}_s), \qquad (32)$$

which entails restrictions on the spectrum of $\bar{J}$.

The analysis of Eq. (32) indicates that mirror symmetry or equivalently Eq. (27) remains a necessary condition for PST in this situation beyond NN couplings. Given mirror symmetry and hence the relation Eq. (21), the PST condition Eq. (32) becomes

$$e^{-i\phi} \exp[-iT Q_M(\bar{x}_s)] = (-1)^{N+s}. \qquad (33)$$

The arguments leading to these results are given below and could be skipped at first read.

Since the right-hand side of Eq. (32) only takes real values, we must have

$$\bar{\chi}_N(\bar{x}_s) = \pm 1 \quad s = 0, 1, \ldots, N. \qquad (34)$$

Let $\{p_k\}$ be a sequence of orthogonal polynomials; for $y_1 < y_2 < \cdots < y_n$ and $z_1 < z_2 < \cdots < z_{n-1}$, the zeros of p_n and p_{n-1}, respectively, it is well known [29] that one has

$$y_1 < z_1 < y_2 < z_2 < \cdots < z_{n-1} < y_n, \qquad (35)$$

a property called the interlacing of the zeros of p_n and p_{n-1}. Applying this result to $\bar{P}_{N+1}$ and $\bar{\chi}_N$, one sees that a zero of $\bar{\chi}_N$ must be encountered between each of the pairs $(\bar{x}_{s-1}, \bar{x}_s)$, $s = 1, 2, \ldots, N$ and, hence, in view of Eq. (34), the sign of $\bar{\chi}_N$ must alternate at successive eigenvalues $\bar{x}_s$. Once this is established, it follows from Eqs. (17) and (20) that we must have $\bar{\chi}_N(\bar{x}_s) = (-1)^{N+s}$ for the weights $\bar{w}_s$ to be positive. This is precisely Eq. (27), which as noted in Sec. II, is tantamount to $\bar{J}$ being mirror-symmetric. We thus conclude that for the special class of chains with non-nearest-neighbor couplings we are considering, a necessary condition for PST is that the underlying Jacobi matrix satisfies $\bar{J} R = R \bar{J}$. This of course

implies that the one-excitation restriction of $Q_M(\bar{J})$ of $H^{(M)}$ itself commutes with R and that the couplings satisfy

$$J_n^{(k)} = J_{N-n+k}^{(k)}, \quad k = 1, \ldots, M.$$
$$B_n = B_{N-n}, \quad k \leqslant n \leqslant N. \qquad (36)$$

Obviously, when $N = 1$, this amounts to Eq. (21), which is known to be one of the necessary conditions for PST when only nearest-neighbor interactions are present. Given the requirement that Eq. (27) be satisfied, condition Eq. (32) becomes Eq. (33), which translates into

$$T Q_M(\bar{x}_s) = -\phi + \pi(N + s + 2L_s) \quad s = 0, \ldots, N, \quad (37)$$

where L_s are arbitrary integers that may depend on s. Equation (37) leads to restrictions on the spectrum of $\bar{J}$ and the coefficients of Q_M; together with the mirror symmetry of $\bar{J}$, it provides the necessary and sufficient conditions for PST in the case under study. In fact, these requirements ensure the full mirror inversion of the one-excitation states after time T. To see this, consider the matrix elements $\langle k|e^{-iTH^{(M)}}|l\rangle$ and use the expansion Eq. (14) over the eigenstates of $\bar{J}$, one has

$$\langle k|e^{-iTH^{(M)}}|l\rangle = \sum_{s=0}^{N} e^{-iT Q_M(\bar{x}_s)} \bar{w}_s \bar{\chi}_k(\bar{x}_s) \bar{\chi}_l(\bar{x}_s). \qquad (38)$$

Using Eq. (33), Eq. (29) and the orthogonality relation Eq. (15) (for the polynomials $\bar{\chi}_n$), one obtains

$$\langle k|e^{-iTH^{(M)}}|l\rangle = e^{i\phi} \sum_{s=0}^{N} \bar{w}_s \bar{\chi}_k(\bar{x}_s) \bar{\chi}_{N-l}(\bar{x}_s)$$
$$= e^{i\phi} \delta_{k,N-l}, \qquad (39)$$

which implies as announced that

$$e^{-iT Q_M(\bar{J})} = e^{i\phi} R. \qquad (40)$$

We shall now further restrict the set of models that we will consider by fixing the matrix $\bar{J}$ and examining PST first for nearest-neighbor and then when next-to-nearest-neighbor couplings are added, that is when $M = 2$.

B. The Krawtchouk chain

The simplest possible spectrum that can be posited for a mirror-symmetric Jacobi matrix is the linear one where

$$\bar{x}_s = s - \frac{N}{2}, \quad s = 0, 1, \ldots, N. \qquad (41)$$

The entries of the corresponding matrix $\bar{J}$ are provided by the coefficients

$$\bar{J}_n = a_n, \quad \bar{B}_n = 0, \qquad (42)$$

with

$$a_n = \frac{1}{2}\sqrt{n(N - n + 1)}. \qquad (43)$$

It is immediate to check that these $\bar{J}_n$ and $\bar{B}_n$ verify Eq. (21) and hence define a mirror-symmetric $\bar{J}$.

The methods of inverse spectral problems can be used to establish the correspondence between the spectrum in Eq. (41) and $\bar{J}$. This matrix can also be obtained through simple

observations that are given in the Appendix, where the name Krawtchouk chain will be justified.

C. The nearest-neighbor case

When $M = 1$ and the Hamiltonian $H^{(1)}$ is defined from Eq. (22) by taking

$$Q_1(\bar{J}) = \beta \bar{J} \tag{44}$$

with β an arbitrary positive real number, it is immediate to recover the well known fact that the Krawtchouk model with nearest-neighbor couplings admits PST. Indeed, condition Eq. (37) reads then

$$T\beta\left(s - \frac{N}{2}\right) = -\phi + \pi(N + s + 2L_s). \tag{45}$$

This shows that the integer numbers L_s must necessarily depend linearly on s and thus take the form $L_s = ls + m$ with l and m integers. With ϕ appropriately chosen to take care of the constant terms, Eq. (45) reveals that PST will be achieved at times T given by

$$T = \frac{\pi}{\beta}(2l + 1) \quad l = 0, 1, \dots \tag{46}$$

Hence, the minimal time for PST in the NN model is $T = \frac{\pi}{\beta}$.

Note that the PST time can be reduced by increasing β but that this comes at the expense of increasing the norm of the Hamiltonian and thus energy in the system. Let us further remark that T (or equivalently β), the time for PST, and the integer N that determines the length of the chain, are treated as two independent parameters. These two quantities are tied together however within the expression for the couplings: $J_n = \frac{\beta}{2}\sqrt{n(N - n + 1)}$. The time T can thus be kept fixed for different N at the expense of changing the Hamiltonian. Note in this connection that the middle couplings grow with N. Therefore, to keep the couplings relatively small, we can either take T proportional to N or, keeping T and N independent, consider chains where N is not too large. The latter view is typically the one adopted with the idea that spin chains are devices aimed at quantum transport over short distances [1].

D. The next-to-nearest-neighbor extension

We are now ready to provide an analytic NNN extension of the Krawtchouk chain and to determine the specifications for which this spin chain will possess PST.

Let $M = 2$ and take $Q_2(\bar{J})$ to be

$$Q_2(\bar{J}) = \alpha \bar{J}^2 + \beta \bar{J}, \tag{47}$$

with α an arbitrary positive real number and β a nonnegative number. According to Eq. (30), $H^{(2)}$ has the following action on the one-excitation states $|n\rangle$:

$$\begin{aligned}
H^{(2)}|n\rangle = &\alpha a_{n+1} a_{n+2}|n + 2\rangle + \beta a_{n+1}|n + 1\rangle \\
&+ \alpha\left(a_n^2 + a_{n+1}^2\right)|n\rangle + \beta a_n|n - 1\rangle \\
&+ \alpha a_{n-1} a_n|n - 2\rangle. \tag{48}
\end{aligned}$$

This defines a spin chain with NNN interactions that extends the Krawtchouk chain with NN links. The couplings and magnetic field strengths of the Hamiltonian $H^{(2)}$ can be read

off from Eq. (48) by comparing it with Eq. (7); one finds

$$J_n^{(1)} = J_n = \beta a_n, \tag{49a}$$

$$J_n^{(2)} = \alpha a_{n-1} a_n. \tag{49b}$$

Note that the NN Hamiltonian $H^{(1)}$ is recovered when $\alpha = 0$, observe moreover that $H^{(2)}$ has magnetic field strengths B_n given by

$$B_n = \alpha\left(a_n^2 + a_{n+1}^2\right), \tag{50}$$

in contrast to $H^{(1)}$, where $B_n = 0$.

The analysis of this NNN model will lead us to results regarding PST that can be summarized as follows. For $\beta > 0$, $H^{(2)}$ will generate PST if $\frac{\alpha}{\beta}$ is a rational number, that is, if $\frac{\alpha}{\beta} = \frac{p}{q}$ where p and q are two co-prime integers. Moreover if p is odd, q and N will need to be of the same parity. PST will then be observed at $T = \frac{\pi q}{\beta}$. For PST to happen in the NNN chain at the same time $\frac{\pi}{\beta}$ as in the NN model, we must have $\frac{\alpha}{\beta} = p$, $p \in \mathbb{N}$, with the odd p only admissible when N is odd. For $\beta = 0$, there will be PST for even N with minimal time $T = \frac{\pi}{\alpha}$, but no PST for odd N.

Let us now explain how this is found by examining if there are values of the parameters α and β for which $H^{(2)}$ will generate PST. The general condition Eq. (37) for PST becomes

$$T\left[\alpha\left(s - \frac{N}{2}\right)^2 + \beta\left(s - \frac{N}{2}\right)\right]$$
$$= -\phi + \pi N + \pi s + 2\pi L_s, \tag{51}$$

when Q_2 is given by Eq. (47). Since the left-hand side of Eq. (51) is a quadratic polynomial in s, we need to take L_s to be also quadratic. Let

$$L_s = \xi s^2 + \eta s + \zeta. \tag{52}$$

It is easy to show that L_s will be an integer for all $s = 0, 1, \dots, N$ when ζ is an integer and ξ and η are simultaneously integers or half-integers. Using Eq. (52) and equating the coefficients of the various powers of s in Eq. (51) leads to the relations

$$\alpha T = 2\pi \xi, \tag{53a}$$

$$2\pi \eta + \pi = -\alpha T N + \beta T, \tag{53b}$$

$$\alpha T \frac{N^2}{4} - \beta \frac{N}{2} = -\phi + \pi N + 2\pi \zeta. \tag{53c}$$

Equation (53c) does not imply any restrictions as it merely provides a relation between the coefficient ζ and the phase ϕ. From Eqs. (53a) and (53b) we see that

$$\frac{\beta}{\alpha} = \frac{2\eta + 1}{2\xi} + N, \tag{54}$$

which indicates that the ratio $\frac{\beta}{\alpha}$ should be a rational number (depending on the choice of ξ and η). From here onwards we will analyze the cases $\beta > 0$ and $\beta = 0$ separately, starting with $\beta > 0$.

The time T for PST is given by

$$T = \frac{2\pi}{\beta}\left[N\xi + \eta + \frac{1}{2}\right]. \tag{55}$$

Because of the limitations on the values of ξ and η, it is clear that only two cases are possible:

$$(i) \quad T = \frac{2\pi j}{\beta},$$

$$(ii) \quad T = \frac{\pi}{\beta}(2j + 1),$$

with j some integer. Indeed, when both ξ and η are integers only case (ii) is realized; when ξ and η are half-integers case (i) occurs when N is even and case (ii) happens when N is odd. The smallest time T for which PST can be obtained arises from case (ii) when $j = 0$. This yields the same minimal PST time as for the NN model which is $T = \frac{\pi}{\beta}$. Equation (55) shows that this implies

$$\eta = -N\xi. \tag{56}$$

When N is odd, Eq. (56) shows that ξ and η can both be chosen to be integers or half-integers. When N is even, then necessarily ξ and η must be integers. Whether N is even or odd, we always have owing to Eq. (56),

$$\frac{\alpha}{\beta} = 2\xi. \tag{57}$$

We thus arrive at the following results. In the NNN chains with parameters α and β, PST is achieved at the same time $T = \frac{\pi}{\beta}$ as in the NN chain (with parameter β) if α is in the following relation with β:

$$(i) \quad \frac{\alpha}{\beta} = 1, 2, 3, \dots \quad \text{for } N \text{ odd}$$

$$(ii) \quad \frac{\alpha}{\beta} = 2, 4, 6, \dots \quad \text{for } N \text{ even}.$$

There are other circumstances when PST can be achieved of course. Recall that Eq. (44) simply required $\frac{\alpha}{\beta}$ to be rational. In general, if $\frac{\alpha}{\beta} = \frac{p}{q}$ where p and q are coprime integers, take

$$\xi = \frac{p}{2} \quad \text{and} \quad \eta = \frac{1}{2}[q - Np - 1], \tag{58}$$

so that $N\xi + \eta + \frac{1}{2} = \frac{q}{2}$ and Eq. (54) is satisfied. If p is even, q must be odd; ξ and η are then both integer. If p is odd, ξ is half-integer; η will also be half-integer either for q odd and N odd or, for q even and N even. In all cases, $T = \frac{\pi q}{\beta}$.

Let us now look at $\beta = 0$, in which case Eqs. (53a) and (53b) yield

$$2\eta + 1 = -2\xi N \tag{59}$$

and

$$T = \frac{2\pi \xi}{\alpha}. \tag{60}$$

Recall that ξ and η are either both integers or both half-integers. In the former case, the left-hand side of Eq. (59) is odd while its right-hand side is even. This contradiction rules out the option ξ, η integers. When ξ and η are both of the form $\xi = u/2$ and $\eta = v/2$ with u and v odd integers, we see that Eq. (59) becomes $u + 1 = -vN$, which can only be fulfilled if N is even. The minimal PST time in this instance is $T = \frac{\pi}{\alpha}$, which is obtained for $\xi = 1/2$.

Note that perfect state transfer will not occur if $\frac{\alpha}{\beta}$ is not rational. This is to be contrasted with the fact that for the NN-Hamiltonian ($\alpha = 0$), PST is always observed. The possibilities of almost perfect state transfer (APST) (see Refs. [30,31]), when $\frac{\alpha}{\beta}$ is irrational remain to be investigated.

It is known that quantum walks generated by spin chains and classical birth and death processes are intimately connected [32]. Let us mention in this respect that our construction of the analytic Hamiltonian $H^{(2)}$ has similarities with the generalization of the Ehrenfest urn model developed in Ref. [28]. This last paper offers an exact solution of a Markov process that involves nearest and next-to-nearest neighbors. Although the analysis in Ref. [28] is framed in terms of matrix orthogonal polynomials, the pentadiagonal one-step transition probability matrix is in fact obtained, up to a constant term, as a quadratic expression with fixed coefficients in the Jacobi matrix of unnormalized Krawtchouk polynomials.

Furthermore, the method proposed in Ref. [33] to produce multiparticle entangled states of ions in an ion trap is based on the use of J_x^2 as Hamiltonian. From our discussion at the end of Sec. III B, we see that this relates to the case $\beta = 0$. The study in Ref. [33] thus has connections to our considerations.

IV. FRACTIONAL REVIVAL

A. General considerations

Fractional revival (FR) can also be observed in certain spin chains. In fact, PST can be viewed as a special case of FR, a phenomenon that sees the time evolution of a wave-packet generate periodically a number of "smaller reproductions" of the initial state at specific locations. In the PST situation, only one unscathed reproduction is observed at given times at the ends of the chain. We shall examine in this section the possibility of FR at two sites in the NNN spin chains on which we have focused so far. To avoid confusion with PST, we shall denote by τ the FR time. FR at the sites 0 and N will be realized at time τ if

$$e^{-iH\tau}|0\rangle = \mu|0\rangle + \nu|N\rangle, \tag{61}$$

where the complex amplitudes μ and ν are subjected to the condition

$$|\mu|^2 + |\nu|^2 = 1. \tag{62}$$

Relation Eq. (61) indicates that the initial state with one spin up at site 0 evolves after time τ into a state that is described by a linear combination of two state vectors associated, respectively, to a spin up at site 0 and another spin up at site N. PST corresponds to $\mu = 0$ ($|\nu| = 1$) and when $\nu = 0$ ($|\mu| = 1$), we have a perfect return. Replacing the entries 0 and 1 by $\uparrow$ and $\downarrow$ in the vectors Eq. (6) (and forgetting the transposition), it is readily recognized that when $\mu = \nu = 1/\sqrt{2}$, the state into which $|0\rangle$ evolves, namely

$$\frac{|0\rangle + |N\rangle}{\sqrt{2}} = \frac{|\uparrow\downarrow \cdots \downarrow\rangle + |\downarrow \cdots \downarrow\uparrow\rangle}{\sqrt{2}},$$

is maximally entangled.

The conditions for fractional revival at two sites in NN spin chains of XX type have been thoroughly analyzed in Ref. [11]. In general, the one-excitation Hamiltonian is only required to

be an isospectral deformation of a mirror-symmetric Jacobi matrix. Here we wish to study the occurrence of FR in spin chains with non-nearest-neighbor interactions that belong to the special class introduced in Sec. II and that have couplings built from polynomials in a mirror-symmetric matrix $\bar{J}$ [see Eq. (30)]. In fact, we want to concentrate in the end on the NNN model with $H^{(2)}|n\rangle = (\alpha \bar{J}^2 + \beta \bar{J})|n\rangle$ and $\bar{J}$ defined by Eqs. (43) and (42), to determine for what values of the parameters α and β will FR occur.

Under the assumption that $\bar{J}$ is mirror-symmetric, the associated polynomials $\bar{\chi}_n(x_s)$ $n = 0,1,\dots,N$ satisfy Eq. (27), that is $\bar{\chi}_N(x_s) = (-1)^{N+s}$. Using the expansion Eq. (14) as in Sec. II and $H^{(M)}|n\rangle = Q_M(\bar{J})|n\rangle$, we see that Eq. (61) amounts to

$$e^{-i\tau Q_M(x_s)} = e^{i\phi}[\mu' + \nu'\bar{\chi}_N(x_s)], \qquad (63)$$

where $\mu = e^{i\phi}\mu'$ and $\nu = e^{i\phi}\nu'$. Note that μ' can be taken real once a global phase term $e^{i\phi}$ has been factored. Taking the modulus of both sides of Eq. (63) and using $\bar{\chi}_N^2(x_s) = 1$, we find that

$$\mathrm{Re}(\mu'\nu') = 0. \qquad (64)$$

Since μ' is taken to be real, ν' must be an imaginary number. In view of Eq. (62), we shall write

$$\mu' = \cos\theta \quad \nu' = i\sin\theta, \qquad (65)$$

and given that $\bar{\chi}_N(x_s) = (-1)^{N+s}$, Eq. (63) will read

$$e^{-i\tau Q_M(x_s)} = e^{i\phi}[\cos\theta + i(-1)^{N+s}\sin\theta]. \qquad (66)$$

In this parametrization, up to integer multiples of π, $\theta = \frac{\pi}{2}$ corresponds to PST and $\theta = 0$ implies a perfect return at time τ.

Let us now focus our attention on the model discussed before with $x_s = s - \frac{N}{2}, s = 0,\dots,N$.

B. The nearest-neighbor Krawtchouk chain

We shall first observe that FR at two sites cannot happen in the Krawtchouk NN model.

Let $M = 1$ with $Q_1(\bar{J}) = \beta \bar{J}$. Condition Eq. (66) becomes

$$e^{-i\tau\beta(s-\frac{N}{2})} = e^{i\phi}[\cos\theta + i(-1)^{N+s}\sin\theta]. \qquad (67)$$

This equation splits into the following two relations according to the parity of s:

$$\beta\tau\left(2s - \frac{N}{2}\right) = -\phi - (-1)^N\theta + 2\pi L_s^{(0)}, \quad (68a)$$

$$\beta\tau\left(2s + 1 - \frac{N}{2}\right) = -\phi + (-1)^N\theta + 2\pi L_s^{(1)}, \quad (68b)$$

where $L_s^{(i)}$, $i = 0,1$, are two *a priori* independent sequences of integers that must be of the form

$$L_s^{(i)} = \gamma_i s + \delta_i, \quad i = 0,1, \qquad (69)$$

with γ_i and δ_i integers. It follows from Eqs. (68a) and (68b) that $\gamma_0 = \gamma_1 = 1,2\dots$ and that

$$\tau = \pi\frac{\gamma_0}{\beta}. \qquad (70)$$

Moreover, apart from a relation determining the phase ϕ in terms of the parameters, one finds that θ is given by

$$\theta = (-1)^N\left[\frac{\gamma_0}{2} + (\delta_0 - \delta_1)\right]\pi. \qquad (71)$$

Therefore, up to sign and integer multiples of π, θ can only take two distinct values, namely 0 and $\frac{\pi}{2}$. This means that only PST and perfect return are possible and as stated at the beginning of this subsection there is no genuine FR.

C. The next-to-nearest-neighbor Krawtchouk chain

We shall here concentrate on the NNN case and find that in contradistinction to the NN situation, balanced FR is possible.

Set $M = 2$ and take $Q_2(\bar{J}) = \alpha \bar{J}^2 + \beta \bar{J}$. If $\alpha \neq 0$, balanced FR will happen if $\frac{\alpha}{\beta} = \frac{p}{q}$ with p and q coprime integers, p odd and N of the same parity as q. We shall now explain how this is obtained.

In view of the expression for $Q_2(\bar{J})$, the FR condition Eq. (66) yields the two relations:

$$\alpha\tau\left(2s - \frac{N}{2}\right)^2 + \beta\tau\left(2s - \frac{N}{2}\right)$$
$$= -\phi - (-1)^N\theta + 2\pi M_s^{(0)}, \qquad (72a)$$
$$\alpha\tau\left(2s + 1 - \frac{N}{2}\right)^2 + \beta\tau\left(2s + 1 - \frac{N}{2}\right)$$
$$= -\phi + (-1)^N\theta + 2\pi M_s^{(1)}, \qquad (72b)$$

where anew, $M_s^{(0)}$ and $M_s^{(1)}$ are sequences of integers. In this case for the two sides of Eqs. (72) to be compatible, we must take quadratic expressions

$$M_s^{(i)} = \xi_i s^2 + \eta_i s + \zeta_i, \quad i = 0,1 \qquad (73)$$

where for each i, independently, ξ_i and η_i can in general be simultaneously integer or half-integer while ζ_i is integer.

Once Eq. (73) is used, equating the coefficients of the powers of s in Eq. (72) gives a system of six equations. It is easy to see that they amount to

$$\xi_0 = \xi_1, \quad \eta_1 - \eta_0 = \xi_0, \qquad (74)$$

$$\xi_0 = \frac{2\alpha\tau}{\pi}, \quad \eta_0 = (\beta - \alpha N)\frac{\tau}{\pi}, \qquad (75)$$

$$\zeta_1 - \zeta_0 = \frac{1}{2\pi}[(\alpha + \beta)\tau - \alpha N\tau - 2(-1)^N\theta], \qquad (76)$$

with the sixth equation fixing the phase ϕ in terms of the parameters α, β, τ, N, θ, ζ_0, and ζ_1.

The relations Eqs. (74) imply that all the parameters ξ_i, η_i, ζ_i, $i = 0,1$ are integers. Indeed, assume that ξ_0 and η_0 are half-integers; $\xi_1 = \xi_0$ and since ξ_1 is hence half-integer, η_1 must also be half-integer. Since the difference $\eta_1 - \eta_0$ of two half-integers is an integer, we have a contradiction with $\eta_1 - \eta_0 = \xi_0$. All parameters can therefore only be integers.

From Eqs. (75), one obtains when $\beta > 0$ the following expression for the FR time τ and the relation Eq. (78) between

α and β:

$$\tau = \frac{\pi}{\beta}\left(\eta_0 + \frac{N}{2}\xi_0\right), \qquad (77)$$

$$\frac{\alpha}{\beta} = \frac{\xi_0}{2\eta_0 + N\xi_0}. \qquad (78)$$

When $\beta = 0$, one gets

$$\tau = \frac{\pi}{2\alpha}\xi_0, \qquad (79)$$

$$\eta_0 = -\frac{N}{2}\xi_0. \qquad (80)$$

From Eq. (76) and using Eq. (65), one finds for θ in both cases

$$\theta = (-1)^N \pi\left[\frac{\xi_0}{4} + \frac{\eta_0}{2} + \zeta_0 - \zeta_1\right]. \qquad (81)$$

We can now draw some conclusions from these formulas on the occurrence of FR in the NNN model.

For $\beta > 0$: (i) First, we find the same constraint on α and β for the presence of FR as for PST, namely that $\frac{\alpha}{\beta}$ is a rational number; (ii) second, we observe that the fractional revival times will be integer multiples of $\frac{\pi}{2\beta}$ which is half the minimal PST time; (iii) third, and most importantly, we note that FR at two sites is genuinely possible. Indeed, up to signs and the addition of integer multiples of π, we see from Eq. (81) that θ can take the values 0, $\frac{\pi}{4}$, $\frac{\pi}{2}$. We already observed that $\theta = 0$ and $\theta = \frac{\pi}{2}$ correspond to perfect return and PST respectively. All possibilities that yield a θ equivalent to $\frac{\pi}{4}$ will give rise, however, to balanced fractional revival where the amplitudes for finding a spin up at the sites 0 and N are both equal in magnitude to $1/\sqrt{2}$. For $\beta = 0$, since ξ_0 and η_0 are integers, Eq. (80) requires N to be even. Therefore: (i) when N is odd no FR occurs; (ii) when N is even θ can be equal to $\frac{\pi}{4}$ modulo multiples of π and FR is possible, in this case the minimal FR time is $\frac{\pi}{2\alpha}$ with PST happening at time $\frac{\pi}{\alpha}$.

The realization of a specific scenario will depend on the characteristics of the NNN model as they are determined by the integer parameters ξ_i, η_i, and ζ_i. From the preceding discussion, we note that FR at sites 0 and N will occur only if ξ_0 is odd. That is, in view of Eq. (78), FR will be seen only in the NNN spin chains where $\frac{\alpha}{\beta} = \frac{p}{q}$ with p and q coprime and p odd. To achieve such a value of $\frac{\alpha}{\beta}$, we may set

$$\xi_0 = p, \quad \eta_0 = \tfrac{1}{2}(q - Np) \qquad (82)$$

to satisfy Eq. (78). Since p is odd, η_0 will be integer as required either when q and N are both even or when q and N are both odd. Irrespective, we see from Eq. (77) that the FR time τ is given by $\tau = \frac{\pi q}{2\beta}$. One observes that this is consistent with the discussion of the conditions for PST; in that case the specifications involved the parameters ξ and η that could be both integers or both half-integers. For p even and q odd, we note that while PST is possible, there will be no FR. The other PST cases will exhibit FR in addition. Comparing Eqs. (58) and (82), we see that

$$\xi = \frac{\xi_0}{2}, \quad \eta = \eta_0 - \tfrac{1}{2}. \qquad (83)$$

Since ξ_0 and η_0 are integers and ξ_0 is odd, this makes ξ and η half-integers in keeping with what was found earlier. Observe

also that the parity considerations on N match. It is then seen that the PST time T is double the FR time τ: $T = 2\tau$.

This last point can also be understood as follows. From Eq. (78), it is clear that we can multiply both parameters ξ_0 and η_0 by the same integer k: $\xi_0 \to k\xi_0, \eta_0 \to k\eta_0$ without changing the ratio $\frac{\alpha}{\beta}$, that is without changing the Hamiltonian essentially. This transformation, however, will have the effect of scaling τ as seen from Eq. (77): $\tau \to k\tau$. Consider now what happens to θ under that transformation when $k = 2$:

$$\theta \to \bar{\theta} = (-1)^{N+1}\pi\left(\frac{\xi_0}{2} + \eta_0 + \zeta_0 - \zeta_1\right). \qquad (84)$$

Assume that we are in a situation of FR and thus that ξ_0 is odd. It follows that $\cos\bar{\theta} = 0$. Such a $\bar{\theta}$ leads to PST since the only nonzero spin-up amplitude is then at site N.

We thus have the following scenario. If fractional revival occurs at time $t = \tau$, then at $t = T = 2\tau$ we shall observe PST, at $t = 3\tau$ fractional revival will be seen again and finally at $t = 2T = 4\tau$ a perfect return will happen. This cycle will then repeat itself with period 4τ.

D. SUMMARY

In this section, we have made the following observations. We have found that while FR does not occur in the NN Krawtchouk spin chain, the presence of additional NNN interactions allow this phenomenon to take place. Furthermore, the only form of FR at sites 0 and N that can be realized is of the balanced type, which corresponds to the generation of a maximally entangled state. Finally, when NN interactions are kept, that is when $\beta > 0$, for FR to occur the parameters α and β of $H^{(2)}$ must satisfy $\frac{\alpha}{\beta} = \frac{p}{q}$ with p and q coprime integers, p odd and q and N both odd or even; FR will then happen at time $\tau = \frac{\pi q}{2\beta}$.

V. CONCLUSION

This paper has provided an analytic spin chain with couplings beyond the nearest neighbors where an exact description of PST and FR could be given. We focused on models where the higher-order interactions are related in a polynomial fashion to those of the nearest neighbors and we concentrated on the one model in that class that extended with NNN links, the simplest nonuniform and well-studied XX spin chain with NN couplings based on angular momentum theory or the recurrence coefficients of the Krawtchouk polynomials. This extended model involves two parameters α and β that tune the intensity of the NNN and NN couplings, respectively. The case $\alpha = 0$ corresponds to the absence of second-order interactions. One recalls that PST is then known to occur first at time $T = \frac{\pi}{\beta}$ and we indicated that no FR is predicted by this most simple model.

When $\alpha \neq 0$ and $\beta \neq 0$, the conditions for PST and FR can be summarized easily. In order for PST to occur, one must have $\frac{\alpha}{\beta} = \frac{p}{q}$ where p and q are coprime integers. Furthermore, if FR is to happen, p must be odd and in that case N must be of the same parity as q.

This NNN model is motivated by the quantum transport in arrays of evanescently coupled wave guides where couplings beyond first order, while generally small, will necessarily

be present. In such experimental realizations [22,23], the distances between the wave guides are adjusted to yield the NN couplings; the formulas in terms of products for the NNN couplings are thus well adapted to this optical waveguide context. Our findings may be interpreted as saying that theoretically FR should occur in photonic lattices and should provide a mechanism for the generation of maximally entangled states. This is in contrast with what the simplest NN Krawtchouk model predicts in this regard. We intend to discuss further the implementation in an optical set up in a future report.

On the theoretical side our study may be extended in many directions. It would be useful to perform various simulations to probe the robustness of the PST and FR phenomena with respect to deviations from the specifications of the analytic model (cf. Ref. [34]). In that regard, it would be worthwhile to explore in details the conditions for almost perfect transfer and fractional revival (cf. Refs. [30,31]). Finally, it would be relevant to construct other NNN analytic models so as to offer experimentalists a wider array of possibilities for tuning and concrete realizations. We plan to pursue some of these questions.

APPENDIX: DERIVATION OF THE KRAWTCHOUK CHAIN

We briefly indicate in this appendix how one can establish that the mirror symmetric Jacobi matrix given by Eqs. (42) and (43) has eigenvalues specified by Eq. (41).

Given Eq. (41), it is seen that $|\bar{P}'_{N+1}(\bar{x}_s)| = s!(N-s)!$. In view of Eq. (26), the weights will be given by the binomial distribution

$$\bar{w}_s = \frac{N!}{s!(N-s)!}\left(\frac{1}{2}\right)^N, \tag{A1}$$

where the normalization constant $N!(\frac{1}{2})^N$ has been determined from $\sum_{s=0}^{N} \bar{w}_s = 1$. The polynomials orthogonal with respect to those weights are known to be the normalized symmetric Krawtchouk polynomials,

$$\hat{K}_n(s) = (-1)^n \sqrt{\binom{N}{n}} {}_2F_1\left[\begin{matrix} -n, -s \\ -N \end{matrix}; 2\right],$$

$$n,s = 0, \ldots, N, \tag{A2}$$

where $\binom{l}{k} = l!/k!(l-k)!$ is the binomial coefficient and ${}_2F_1$ is the hypergeometric series

$$ {}_2F_1\left[\begin{matrix} a,b \\ c \end{matrix}; z\right] = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} \frac{z^k}{k!}, \tag{A3}$$

with $(a)_k$ the Pochhammer symbol defined by

$$(a)_0 = 1 \quad (a)_k = a(a+1)\ldots(a+k-1),$$
$$k = 1,2,\ldots \tag{A4}$$

Note that ${}_2F_1[\begin{smallmatrix} a,b \\ c \end{smallmatrix}; z]$ terminates when a or b is a negative integer. One has

$$\sum_s \frac{N!}{s!(N-s)!}\left(\frac{1}{2}\right)^N \hat{K}_m(s)\hat{K}_n(s) = \delta_{nm}. \tag{A5}$$

Now it can be checked directly or by consulting Ref. [35] that these polynomials $\hat{K}_n(s)$ satisfy the three-term recurrence relation

$$\left(s - \frac{N}{2}\right)\hat{K}_n(s) = a_{n+1}\hat{K}_{n+1}(s) + a_n \hat{K}_{n-1}(s), \tag{A6}$$

with a_n given by Eq. (43). With $\bar{\chi}_n(\bar{x}_s)$ identified as $\hat{K}_n(s)$, this implies that the entries of the matrix $\bar{J}$ coincide with Eq. (42).

Alternatively, one can also use quantum angular momentum theory to relate the spectrum Eq. (41) to the matrix $\bar{J}$ with elements given by Eqs. (43) and (42). Indeed, observe that this $(N+1)$-dimensional matrix $\bar{J}$ coincides with that of the angular momentum operator J_x in the standard basis $|j,m\rangle = |\frac{N}{2}, s - \frac{N}{2}\rangle$, $s = 0, \ldots, N$, where the z-projection J_z is diagonalized : $J_z|j,m\rangle = m|j,m\rangle$. Since all angular momentum components have the same spectrum, it follows that $\bar{J}$ has Eq. (41), that is $(-\frac{N}{2}, -\frac{N}{2}+1, \ldots, \frac{N}{2}-1, \frac{N}{2})$ as eigenvalues. Now the eigenvectors of J_x are obtained by transforming the vectors $|j,m\rangle$ under a rotation that takes the z axis into the x axis. Since elements of matrices irreducibly representing rotations are expressed in terms of Krawtchouk polynomials [36], their occurrence in our problem is thus understood.

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