Quantum communication and state transfer in spin chains

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Abstract. We investigate the time evolution of a single spin excitation state in certain linear spin chains, as a model for quantum communication. We consider first the simplest possible spin chain, where the spin chain data (the nearest neighbour interaction strengths and the magnetic field strengths) are constant throughout the chain. The time evolution of a single spin state is determined, and this time evolution is illustrated by means of an animation. Some years ago it was discovered that when the spin chain data are of a special form so-called perfect state transfer takes place. These special spin chain data can be linked to the Jacobi matrix entries of Krawtchouk polynomials or dual Hahn polynomials. We discuss here the case related to Krawtchouk polynomials, and illustrate the possibility of perfect state transfer by an animation showing the time evolution of the spin chain from an initial single spin state. Very recently, these ideas were extended to discrete orthogonal polynomials of q-hypergeometric type. Here, a remarkable result is a new analytic model where perfect state transfer is achieved: this is when the spin chain data are related to the Jacobi matrix of q-Krawtchouk polynomials. This case is discussed here, and again illustrated by means of an animation.

1. Introduction

The transfer of a quantum state (i.e. a qubit) from one site to another is a key requirement in quantum communication. This process is important for connecting distinct quantum processors or for the (short distance) mapping of quantum states to elements of a quantum register.

S. Bose [1, 2] introduced linear spin chains as a channel for such short distance quantum communication. An excellent review paper on the topic was published in 2007 [3]. Since the pioneering work of Bose, the study of transmission of data in such linear quantum registers has been the subject of many investigations [1, 4, 5, 6, 7].

The linear spin chains as introduced by Bose consist of a linear sequence of permanently coupled qubits, i.e. quantum two-state systems. These are realized as spin-1/2 systems, where $|0\rangle$ is the notation for spin down and $|1\rangle$ for spin up. The question is whether the chain can act as a quantum data-bus if the interactions in the chain are permanent (i.e. the couplings are always "on" and fixed in strength).

From the mathematical point of view, a linear spin chain is determined by its Hamiltonian. A system of $N+1$ interacting qubits (spin 1/2 particles) in a quantum register is usually modeled by an isotropic Hamiltonian of XY type:

$$\hat{H} = \frac{1}{2}\sum_{k=0}^{N-1} J_k(\sigma_k^x \cdot \sigma_{k+1}^x + \sigma_{k+1}^y \cdot \sigma_k^y) + \frac{1}{2}\sum_{k=0}^{N} h_k(\sigma_k^z + 1), \tag{1}$$

where J_k is the coupling strength between the kth and $(k+1)$th qubit, and h_k is the "Zeeman" energy of the kth qubit. For such Hamiltonians, it is common to use the Jordan-Wigner transformation, mapping the Pauli matrices to spinless lattice fermions [8, 9]. Then the Hamiltonian takes the form

$$\hat{H} = \sum_{k=0}^{N-1} J_k(a_k^\dagger a_{k+1} + a_{k+1}^\dagger a_k) + \sum_{k=0}^{N} h_k a_k^\dagger a_k. \tag{2}$$

We shall be dealing with the problem in this form; the constants J_k and h_k are referred to as the spin chain data.

Initially, the system is in its completely polarized ground state $|\mathbf{0}\rangle = |00\cdots 0\rangle = |0\rangle\otimes|0\rangle\otimes\cdots\otimes|0\rangle$, where $|0\rangle$ denotes the spin down state. Let $|k) = |00\cdots 010\cdots 0\rangle = a_k^\dagger|\mathbf{0}\rangle$ $(k = 0, 1, \ldots, N)$ denote a state in which there is a single fermion at the site k and all other sites are empty, i.e. $|k)$ describes the state in which the spin at the site k has been flipped to $|1\rangle$. These notions are illustrated in the following figures.

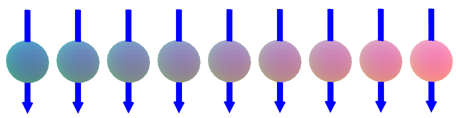

Figure 1. Illustration of the ground state $|\mathbf{0}\rangle$ of the linear spin chain, with all spins down.

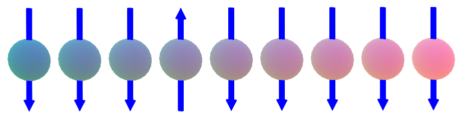

Figure 2. Illustration of the single fermion state $|k)$, with the spin at site k up and all others down (here $k = 3$).

The set of states $|k)$ $(k = 0, 1, \ldots, N)$ forms a basis for the single-fermion states of the system. In this single-fermion basis, the Hamiltonian $\hat{H}$ takes the matrix form

$$M = \begin{pmatrix} h_0 & J_0 & 0 & \cdots & 0 \\ J_0 & h_1 & J_1 & \cdots & 0 \\ 0 & J_1 & h_2 & \ddots & \\ \vdots & \vdots & \ddots & \ddots & J_{N-1} \\ 0 & 0 & & J_{N-1} & h_N \end{pmatrix}. \tag{3}$$

The dynamics (time evolution) of the system is completely determined by the eigenvalues ϵ_j and eigenvectors φ_j of this matrix M. Once the single-fermion eigenstates φ_j are determined, the n-fermion eigenstates of $\hat{H}$ $(n \le N)$ can be constructed using the technique of Slater determinants [9, 10]. In order to determine the single-fermion states, note that the matrix M in (3) is real and symmetric, so the spectral theorem [11] implies that it can be written as $M = UDU^T$, where D is a diagonal matrix and U an orthogonal matrix:

$$D = \mathrm{diag}(\epsilon_0, \epsilon_1, \ldots, \epsilon_N), \tag{4}$$
$$UU^T = U^T U = I. \tag{5}$$

The entries of D are the single-fermion energy eigenvalues, and the columns of the matrix U are the (orthonormal) eigenvectors of M, i.e. the single-fermion eigenstates $\varphi_j = \sum_{k=0}^{N} U_{kj}\,|k)$ with $\hat{H}\varphi_j = M\varphi_j = \epsilon_j\,\varphi_j$.

The *dynamics* of the system under consideration is described by the unitary time evolution operator $\mathcal{U}(t) \equiv \exp(-it\hat{H})$. Assume that the "state sender" is located at site s of the spin chain, and the "state receiver" at site r (s and r are site labels, belonging to $\{0,1,\ldots,N\}$). At time $t=0$ the sender turns the system into the single spin state $|s)$. After a certain time t, the system evolves to the state $\mathcal{U}(t)|s)$ which may be expressed as a linear superposition of all the single spin states. So the transition amplitude of an excitation from site s to site r of the spin chain is given by the time-dependent correlation function

$$f_{r,s}(t) = (r|\mathcal{U}(t)|s). \tag{6}$$

Using the orthogonality of the states φ_j, one finds [12]:

$$f_{r,s}(t) = \langle \sum_{k=0}^{N} U_{rk}\varphi_k|\exp(-it\hat{H})\sum_{j=0}^{N} U_{sj}\varphi_j\rangle = \sum_{j=0}^{N} U_{rj}U_{sj}e^{-it\epsilon_j}. \tag{7}$$

One says that there is *perfect state transfer* at time t from one end of the chain to the other end when $|f_{N,0}(t)| = 1$. The conditions for perfect state transfer can quite easily be described in terms of the "mirror symmetry" of the matrix M in (3), see [13, 7]. However, if our aim is to study analytical solutions, we should also require the conditions that the eigenvalues ϵ_j and the eigenvector components U_{kj} should be analytic (closed form) expressions, for arbitrary N (i.e. the value of N is not fixed, and appears as a parameter in the closed form expressions of ϵ_j and U_{kj}). We shall refer to such cases as "analytically solvable Hamiltonians $\hat{H}$".

The purpose of this contribution is to present some results and examples of spin chains allowing perfect state transfer in the context of orthogonal polynomials. These examples are taken from [12] and [14]. The main addition for the current contribution is that we present some animations illustrating the ideas of perfect state transfer in this context.

2. Spin chain with constant interaction

The simplest possible example of a Hamiltonian $\hat{H}$ that is analytically solvable has zero background magnetic field (i.e. all $h_k = 0$) and constant nearest-neighbour interaction in the chain (i.e. all $J_k = 1$). For an interaction matrix M with these simple spin chain data, there is indeed an analytically closed form expression for its eigenvalues and eigenvectors [1]. In particular,

$$\epsilon_j = 2\cos\left(\frac{(j+1)\pi}{N+2}\right), \qquad (j = 0,1,\ldots,N) \tag{8}$$

and the eigenvectors φ_j are the columns of the (orthogonal) matrix U given by

$$U_{ij} = \sqrt{\frac{2}{N+2}}\sin\left(\frac{(i+1)(j+1)\pi}{N+2}\right) \qquad (i,j = 0,1,\ldots,N). \tag{9}$$

Following (7), the correlation function becomes

$$f_{r,s}(t) = \sum_{j=0}^{N}\frac{2}{N+2}\sin\left(\frac{(r+1)(j+1)\pi}{N+2}\right)\sin\left(\frac{(s+1)(j+1)\pi}{N+2}\right)\exp\left(-2it\cos\left(\frac{(j+1)\pi}{N+2}\right)\right). \tag{10}$$

Let us consider this function in more detail for the case $s = 0$ (i.e. the sender is at the left end of the chain). For any time t, one can compute the function $f_{r,0}(t)$ or its absolute value $|f_{r,0}(t)|$, and this for all r-values ($r = 0, 1, \ldots, N$). If $|f_{r,0}(t)| = 0$, the rth spin of the system is spin down (depicted by an arrow down for site r). If $|f_{r,0}(t)| = 1$, the rth spin of the system is spin up (depicted by an arrow up). In general, when $0 < |f_{r,0}(t)| < 1$, the rth spin of the system is in a superposition state of the form

$$\cos(\alpha)|0\rangle + e^{i\phi}\sin(\alpha)|1\rangle.$$

Such a state can be depicted by an arrow in the direction of the angle α; following our convention of spin up and spin down, this means $\alpha = -\frac{\pi}{2} + \pi|f_{r,0}(t)|$.

We are now in a position to illustrate the time evolution of such a spin chain by means of an animation. Consider the spin chain with $N = 8$. In the following figure, we depict the evolution of the system for time t running from 0 to 3π. At time $t = 0$, the system is in the initial state $|0)$ with the leftmost spin in a pure state with spin up, and all the others spin down. Then, at any time t, we compute $f_{r,0}(t)$ for $r = 0, 1, \ldots, N$, and depict the corresponding arrows according to the above-mentioned convention. The result is shown in Figure 3, as an animation.

In this case, due to the nature of the correlation function $f_{r,0}(t)$ given by (10), there is clearly no perfect state transfer. In other words, at any time $t > 0$ all values $f_{r,0}(t)$ satisfy $0 < |f_{r,0}(t)| < 1$.

animation1

Figure 3. Time evolution of a linear spin chain with constant data. Click on the picture to see the animation running, from $t = 0$ up to $t = 3\pi$. This movie is also available as animation1.gif in the *Supplementary Data* accompanying this paper.

3. Spin chains allowing perfect state transfer

The previous example did not allow perfect state transfer, due to the simple choice of the spin chain data. It is known, however, that if the spin chain data J_k and h_k are chosen appropriately, perfect state transfer is possible. Such an example was given in [10, 4], with spin chain data

$$h_k = N/2, \qquad J_k = \frac{1}{2}\sqrt{(k+1)(N-k)}. \tag{11}$$

It turns out that in this case, the eigenvectors of M are related to Krawtchouk polynomial evaluations. For a second known example allowing perfect state transfer [10], dual Hahn polynomials play a role. In this context, we studied more generally systems where the spin chain data is related to the Jacobi matrix of a set of discrete orthogonal polynomials [12]. This general approach also leads to closed form expressions for the correlation function $f_{r,s}(t)$.

Let us present one example here, based upon the Krawtchouk polynomials. The Krawtchouk polynomial of degree n ($n = 0, 1, \ldots, N$) in the variable x, with parameter $0 < p < 1$ is given by

$$K_n(x) \equiv K_n(x; p, N) = {}_2F_1\left[\begin{array}{c} -x, -n \\ -N \end{array}; \frac{1}{p}\right]. \tag{12}$$

The function ${}_2F_1$ is the classical hypergeometric series [15, 16], and in this case it is a terminating series because of the appearance of the negative integer $-n$ as a numerator parameter. Krawtchouk polynomials satisfy a (discrete) orthogonality relation [17]:

$$\sum_{x=0}^{N} w(x) K_n(x) K_m(x) = d_n \delta_{mn}, \tag{13}$$

where $w(x)$ is the weight function in x and d_n is a function depending on n:

$$w(x) = \binom{N}{x} p^x \,(1-p)^{N-x} \qquad (x = 0, 1, \ldots, N); \qquad\qquad d_n = \frac{1}{\binom{N}{n}} \left(\frac{1-p}{p} \right)^n . \tag{14}$$

They also satisfy the following three-term recurrence relation:

$$-\, x K_n(x) = n(1-p)\, K_{n-1}(x) - \big[p(N-n) + n(1-p)\big]\, K_n(x) + \, p(N-n)\, K_{n+1}(x). \tag{15}$$

It is convenient to introduce orthonormal Krawtchouk functions by

$$\tilde{K}_n(x) \equiv \frac{\sqrt{w(x)} K_n(x)}{\sqrt{d_n}}, \tag{16}$$

satisfying

$$x \tilde{K}_n(x) = J_{n-1}\, \tilde{K}_{n-1}(x) + h_n\, \tilde{K}_n(x) + J_n\, \tilde{K}_{n+1}(x), \tag{17}$$

where

$$h_n = Np + (1-2p)n, \qquad J_n = -\sqrt{p(1-p)}\sqrt{(n+1)(N-n)}. \tag{18}$$

In other words, for the interaction matrix M_K with the above spin chain data, and a matrix U with $U_{jk} = \tilde{K}_j(k)$, one has $M_K U = UD$, where $D = \mathrm{diag}(0, 1, 2, \ldots, N)$ (due to the recurrence relation), and U is an orthogonal matrix (due to the orthogonality relations of the polynomials). So the eigenvectors of the Hamiltonian (in the single-fermion case) corresponding to the quantities (18) have components equal to normalized Krawtchouk polynomials, and the corresponding energy eigenvalues are $\epsilon_k = k$ $(k = 0, 1, \ldots, N)$. This implies that the correlation function (7), where we put $z = e^{-it}$, takes the following form:

$$\begin{aligned} f_{r,s}(t) &= \sum_{k=0}^{N} U_{rk} U_{sk} z^{\epsilon_k} = \sum_{k=0}^{N} \tilde{K}_r(k) \tilde{K}_s(k) z^k \\ &= \frac{1}{\sqrt{d_r d_s}} \sum_{k=0}^{N} w(k) K_r(k) K_s(k) z^k \qquad (z = e^{-it}). \end{aligned} \tag{19}$$

Now one can use summation formulas for hypergeometric series, leading to [12]

$$\begin{aligned} f_{r,s}(t) &= \sqrt{\binom{N}{r}\binom{N}{s}} (\sqrt{p(1-p)})^{r+s} (1-z)^{r+s} (1-p+pz)^{N-r-s} \\ &\quad \times {}_2F_1 \left[\begin{matrix} -r, -s \\ -N \end{matrix} ; \frac{-z}{p(1-p)(1-z)^2} \right]. \end{aligned} \tag{20}$$

This is a closed form expression for the general correlation function. Note that it can also be obtained by means of a group theoretical computation [12]: the Jacobi matrix M_K can be identified with an element of the Lie algebra $su(2)$ in the $(N+1)$-dimensional representation. Then the calculation of

$$f_{r,s}(t) = (r|\exp(-itM_K)|s)$$

simply leads to the computation of a matrix element of an $SU(2)$ group element, and these are known as d-functions, related to Jacobi polynomials, i.e. expressed as ${}_2F_1$-functions [18, Chapter 4].

Let us now consider the possibility of perfect state transfer. From (20), one finds

$$f_{N,0}(t) = \left(\sqrt{p(1-p)}\right)^N (1-e^{-it})^N, \tag{21}$$

so in particular $f_{N,0}(\pi) = 1$ when $p = 1/2$. In other words, this model allows perfect state transfer when the parameter $p = 1/2$, and the transfer takes place at time $t = \pi$. This is illustrated as an animation in Figure 4.

animation2

Figure 4. Time evolution of a linear spin chain ($N = 8$) with data determined by the Jacobi matrix of Krawtchouk polynomials (18). Here $p = 1/2$. Click on the picture to see the animation running, from $t = 0$ up to $t = \pi$. Note that there is indeed perfect state transfer. (view as animation2.gif in *Supplementary Data*)

When the parameter p is different from 1/2, one can see from (21) that $|f_{N,0}(t)|$ never reaches the value 1. Once again, let us illustrate this as an animation, see Figure 5. Note that at time $t = 2\pi$ the system is back in its initial state. This is because in general the function (19) is a periodic function with period 2π.

animation3

Figure 5. Time evolution of a linear spin chain ($N = 8$) with data determined by the Jacobi matrix of Krawtchouk polynomials (18). Now we have chosen $p = 1/3$. Click on the picture to see the animation running, from $t = 0$ up to $t = 2\pi$, and note that there is no perfect state transfer. (view as animation3.gif in *Supplementary Data*)

It should be mentioned that general conditions for perfect state transfer can be set up in terms of the interaction matrix M [4, 10, 7]. Following this, one can in principle use a numerical procedure known as the inverse eigenvalue problem, and design spin chains for perfect state transfer numerically [13]. This is, however, always for a chosen numerical value of N, whereas here we have worked with arbitrary N.

In [12] systems for which the interaction matrix coincides with the Jacobi matrix of a set of orthogonal polynomials were systematically investigated. Although no other solutions with perfect state transfer were found this way, the theoretical analysis gave rise to a number of interesting results: explicit formulas for transition amplitudes (or correlation functions), an explanation of why these two systems discovered in [10] are so special, and a group theoretical approach of the problem. For the case where the Jacobi matrix coincides with that of Krawtchouk polynomials (described above), some interesting limiting cases were also discussed in [12]. When the Jacobi matrix is that of Hahn polynomials (then two parameters α and β are involved), a compact formula for $f_{r,s}(t)$ was obtained, but no perfect state transfer is possible (although there were interesting limiting cases). When the Jacobi matrix is that of dual Hahn polynomials (with two parameters γ and δ), again a compact formula for $f_{r,s}(t)$ was obtained. This time, perfect state transfer is possible when $\gamma = \delta = \frac{2P+1}{2Q}$, $P, Q \in \mathbb{N}$, at time $t = Q\pi$. This corresponds to the second example of [10]. Note that in this case the single-fermion energy eigenvalues are of the form $\epsilon_k = k(k + \gamma + \delta + 1)$. Finally, when the Jacobi matrix is that of Racah polynomials (now four parameters α, β, γ and δ are present), a (more complicated) formula for $f_{r,s}(t)$ was obtained, but no new transfer results compared to earlier cases followed.

4. Spin chains with q-numbers in the spin chain data

The approach of spin chains with data originating from Jacobi polynomials of discrete orthogonal polynomials, as initiated in [12], turned out to be very illuminating. Apart from several known systems of discrete orthogonal polynomials of hypergeometric type in the Askey-scheme [17], there is also a list of discrete orthogonal polynomials of q-hypergeometric type. So it is a natural question to ask whether Jacobi matrices of these q-orthogonal polynomials could also function as interaction matrices for spin chains, and whether they would give rise to new solutions with perfect state transfer. This topic was treated in [14]. Among the main results there is indeed a new analytical solution for a spin chain with perfect state transfer. This new solution occurs in the context of q-Krawtchouk polynomials. In [14] all cases of the q-Askey-scheme were studied, and their analysis has shown that this is the only new case with perfect state transfer. For the complete analysis, we refer to [14]. Here, we shall just present the simple case related to q-Krawtchouk polynomials, that leads to a new model for perfect state transfer.

Let us first fix some notation. In the context of q-series, q is a positive real number with $q \neq 1$, and for us it can be considered as an extra parameter in the model. We use the common notation for q-numbers:

$$[n] \equiv [n]_q = \frac{1-q^n}{1-q} \qquad (n \in \mathbb{Z}) \tag{22}$$

and $[n] \to n$ in the limit $q \to 1$. For any complex number a and any nonnegative integer n, the q-shifted factorial is defined by

$$(a;q)_n = (1-a)(1-aq)\cdots(1-aq^{n-1}), \tag{23}$$

and the product is just 1 when $n = 0$. Sometimes, in the context when $0 < q < 1$, one also uses the infinite product

$$(a;q)_\infty = \prod_{k=0}^{\infty}(1-aq^k). \tag{24}$$

For products of q-shifted factorials, it is common to use the abbreviation

$$(a_1, a_2, \ldots, a_A; q)_n = (a_1;q)_n(a_2;q)_n\cdots(a_A;q)_n. \tag{25}$$

The q-hypergeometric series or *basic hypergeometric series* ${}_A\phi_B$ depends on A numerator parameters a_i, B denominator parameters b_i and a variable z and is defined as [19]:

$$ {}_A\phi_B \left[\begin{array}{c} a_1, a_2, \ldots, a_A \\ b_1, \ldots, b_B \end{array} ; q, z \right] = \sum_{n=0}^{\infty} \frac{(a_1, a_2, \ldots, a_A; q)_n}{(q, b_1, \ldots, b_B; q)_n} \left[(-1)^n q^{\binom{n}{2}} \right]^{1+B-A} z^n. \tag{26} $$

When the numerator contains a parameter of the form q^{-m}, with m a nonnegative integer, the series is terminating.

The q-Krawtchouk polynomials $\mathcal{K}_n(q^{-x}; p, N; q)$ are characterized by a positive integer parameter N and a positive real parameter p: $p > 0$. This polynomial of degree n in q^{-x} is defined as [17]

$$ \mathcal{K}_n\left(q^{-x}\right) \equiv \mathcal{K}_n(q^{-x}; p, N; q) = {}_3\phi_2 \left[\begin{array}{c} q^{-n}, q^{-x}, -pq^n \\ q^{-N}, 0 \end{array} ; q, q \right], \qquad n = 0, 1, \ldots, N. \tag{27} $$

The q-Krawtchouk polynomials satisfy a discrete orthogonality relation, namely

$$ \sum_{x=0}^{N} w(x) \mathcal{K}_m(q^{-x}) \mathcal{K}_n(q^{-x}) = d_n \delta_{mn}, \tag{28} $$

where the weight function is

$$ w(x) = \frac{(q^{-N}; q)_x}{(q; q)_x} (-p)^{-x}, \tag{29} $$

and the square norm is

$$ d_n = \frac{(q, -pq^{N+1}; q)_n}{(-p, q^{-N}; q)_n} \frac{(1+p)}{(1+pq^{2n})} (-pq; q)_N \, p^{-N} q^{-\binom{N+1}{2}} (-pq^{-N})^n q^{n^2}. \tag{30} $$

It is easy to see that $d_n > 0$ for $0 < q < 1$ and also for $q > 1$ (since $p > 0$). The polynomials $\mathcal{K}_n(q^{-x})$ also satisfy the following three term recurrence relation:

$$ -(1 - q^{-x}) \mathcal{K}_n(q^{-x}) = A_n \mathcal{K}_{n+1}(q^{-x}) - (A_n + C_n) \mathcal{K}_n(q^{-x}) + C_n \mathcal{K}_{n-1}(q^{-x}), \tag{31} $$

with [17]

$$ A_n = \frac{(1 - q^{n-N})(1 + pq^n)}{(1 + pq^{2n})(1 + pq^{2n+1})}, \qquad C_n = -pq^{2n-N-1} \frac{(1 + pq^{n+N})(1 - q^n)}{(1 + pq^{2n-1})(1 + pq^{2n})}. \tag{32} $$

The corresponding orthonormal q-Krawtchouk functions

$$ \tilde{\mathcal{K}}_n(q^{-x}) \equiv \sqrt{\frac{w(x)}{d_n}} \mathcal{K}_n(q^{-x}) \tag{33} $$

satisfy the recurrence relation

$$ -[-x] \tilde{\mathcal{K}}_n(q^{-x}) = J_{n-1} \tilde{\mathcal{K}}_{n-1}(q^{-x}) + h_n \tilde{\mathcal{K}}_n(q^{-x}) + J_n \tilde{\mathcal{K}}_{n+1}(q^{-x}), \tag{34} $$

where

$$ J_n = \frac{A_n}{1-q} \sqrt{\frac{d_{n+1}}{d_n}}, \qquad h_n = -\frac{A_n + C_n}{1-q}. \tag{35} $$

As in the previous section, for the interaction matrix M_{qK} with the above spin chain data, and a matrix U with $U_{jk} = \tilde{\mathcal{K}}_j(q^{-k})$, one has $M_{qK}U = UD$, where $D = \mathrm{diag}(\epsilon_0, \epsilon_1, \epsilon_2, \dots, \epsilon_N)$ with $\epsilon_k = -[-k]$ (due to the recurrence relation), and U is an orthogonal matrix (due to the orthogonality relations of the polynomials). In other words, the eigenvectors of the Hamiltonian (in the single-fermion case) corresponding to the quantities (35) have components equal to normalized q-Krawtchouk polynomials, and the corresponding energy eigenvalues are

$$\epsilon_k = -[-k] = -\frac{1-q^{-k}}{1-q} = q^{-1} + q^{-2} + \cdots + q^{-k}. \tag{36}$$

As before, the correlation function becomes

$$f_{r,s}(t) = \sum_{k=0}^{N} U_{rk}U_{sk}z^{\epsilon_k} = \frac{1}{\sqrt{d_r d_s}} \sum_{k=0}^{N} w(k)\mathcal{K}_r(q^{-k})\mathcal{K}_s(q^{-k})z^{-[-k]} \qquad (z = e^{-it}). \tag{37}$$

In order to evaluate this sum, consider first the simple case when sender and receiver are at different ends of the chain, namely when $s = 0$ and $r = N$. One finds:

$$\sum_{k=0}^{N} w(k)\mathcal{K}_N(q^{-k})\mathcal{K}_0(q^{-k})z^{-[-k]} = \sum_{k=0}^{N} \frac{(q^{-N};q)_k}{(q;q)_k} q^{Nk} z^{-[-k]}. \tag{38}$$

Because of the factor $z^{-[-k]}$, the sum in (38) is not of q-hypergeometric type, hence there is no hope that it can be simplified any further for arbitrary values of z (i.e. for arbitrary values of t). For certain specific values, however, simplification does take place. Since $z = e^{-it}$, one has

$$z^{-[-k]} = e^{-it(q^{-1}+q^{-2}+\cdots+q^{-k})}.$$

Assume now that the deformation parameter q is a rational number of the following form:

$$q^{-1} = \frac{P}{Q}, \quad \text{with } P \text{ and } Q \textit{ odd} \text{ positive integers (having no common factors).} \tag{39}$$

Then, for each value of the index k with $k \le N$:

$$\begin{aligned} q^{-1} + q^{-2} + \cdots + q^{-k} &= \frac{1}{Q^N}(PQ^{N-1} + P^2Q^{N-2} + \cdots + P^kQ^{N-k}) \\ &= \frac{1}{Q^N} \times k \times (\text{an odd integer}). \end{aligned} \tag{40}$$

Suppose now that we consider the system at time

$$t = T \equiv Q^N \pi,$$

then

$$z^{-[-k]} = e^{-it(q^{-1}+q^{-2}+\cdots+q^{-k})} = e^{-i\pi(PQ^{N-1}+P^2Q^{N-2}+\cdots+P^kQ^{N-k})} = (-1)^k.$$

In this case, the expression (38) simplifies drastically, since on can apply the q-binomial theorem [19, (II.4)]:

$$\sum_{k=0}^{N} \frac{(q^{-N};q)_k}{(q;q)_k} q^{Nk}(-1)^k = (-1;q)_N = \prod_{j=0}^{N-1}(1+q^j). \tag{41}$$

Taking into account the expressions for d_0 and d_N from (30), one has

$$f_{N,0}(T) = \frac{(-1;q)_N}{\sqrt{d_0 d_N}} = (-1;q)_N \sqrt{\frac{p^N q^{N(N+1)/2}}{(-pq, -pq^N; q)_N}}.$$

It is easy to see that this expression takes its maximum value when $p = q^{-N}$, and in that case

$$f_{N,0}(T)\Big|_{p=q^{-N}} = \sqrt{\frac{q^{-N(N-1)/2}(-1;q)_N}{(-q^{-N+1};q)_N}} = 1,$$

allowing perfect state transfer. So the q-Krawtchouk polynomials with parameter $p = q^{-N}$ and q of the special form (39) yield a new model of a spin chain with perfect state transfer.

Once again, let us illustrate this as an animation, see Figure 6.

animation4

Figure 6. Time evolution of a linear spin chain ($N = 8$) with data determined by the Jacobi matrix of q-Krawtchouk polynomials. Here $p = q^{-N} = q^{-8}$, and $q = Q/P = 3$. Click on the picture to see the animation running, from $t = 0$ up to $t = T = Q^N\pi = 3^8\pi$. Note that there is perfect state transfer. (view as animation4.gif in *Supplementary Data*)

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References

[1] Bose S 2003 *Phys. Rev. Lett.* **91** 207901
[2] Bose S, Jin B-Q and Korepin V E 2005 *Phys. Rev. A* **72** 022345
[3] Bose S 2007 *Contemp. Phys.* **48** 13
[4] Christandl M, Datta N, Ekert A and Landahl A J 2004 *Phys. Rev. Lett.* **92** 187902
[5] Christandl M, Datta N, Dorlas T C, Ekert A, Kay A and Landahl A J 2005 *Phys. Rev. A* **71** 032312
[6] Paternostro M, Palma G M, Kim M S and Falci G 2005 *Phys. Rev. A* **71** 042311
[7] Kay A 2009 A review of perfect state transfer and its application as a constructive tool (*Preprint* arXiv:0903.4274v2).
[8] Jordan P and Wigner E 1928 *Z. Phys.* **47** 631
[9] Lieb E and Wu F 1968 *Phys. Rev. Lett.* **20** 1445-1448
[10] Albanese C, Christandl M, Datta N and Ekert A 2004 *Phys. Rev. Lett.* **93** 230502
[11] Golub G H and Van Loan C F 1996 *Matrix Computations* (Baltimore: Johns Hopkins University Press)
[12] Chakrabarti R and Van der Jeugt J 2010 *J. Phys. A* **43** 085302
[13] Karbach P and Stolze J 2005 *Phys. Rev. A* **72** 030301
[14] Jafarov E I and Van der Jeugt J 2010 *J. Phys. A* **43** 405301
[15] Bailey W N 1964 *Generalized hypergeometric series* (Cambridge: Cambridge University Press)
[16] Slater L J 1966 *Generalized hypergeometric functions* (Cambridge: Cambridge University Press)
[17] Koekoek R, Lesky P A and Swarttouw R F 2010 *Hypergeometric orthogonal polynomials and their q-analogues* (Berlin: Springer)
[18] Edmonds A R 1960 *Angular momentum in quantum theory* (Princeton: Princeton University Press)
[19] Gasper G and Rahman M 2004 *Basic hypergeometric series* (Cambridge: Cambridge University Press)