CLASSIFICATION OF SOLVABLE MIRROR-PERIODIC QUANTUM SPIN CHAINS

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Abstract. We present a classification scheme for mirror periodic quantum spin chains with nearest neighbor couplings whose eigenstates can be expressed in analytically closed form in terms of hypergeometric polynomials. These chains of arbitrary finite length exhibit a strong state transfer property, according to which the mirror image of a state is periodically reconstituted. We also construct their continuous space limit using the limit relations between hypergeometric polynomials in the Askey scheme.

1. Introduction

Applications to quantum information theory have motivated the interest in the design of quantum spin chains that implement interesting logic operations. In a recent paper [1], Albanese et al. have considered the problem of engineering a chain able to execute the operation of *mirror inversion*. More precisely, the authors considered a quantum spin chain with nearest neighbor couplings whose Hamiltonian can be written as follows in the spin representation:

$$\mathbb{H} = \frac{1}{2}\sum_{x=0}^{N-1} J_x \left(\sigma_x^{(1)} \cdot \sigma_{x+1}^{(1)} + \sigma_x^{(2)} \cdot \sigma_{x+1}^{(2)}\right) + \frac{1}{2}\sum_{x=0}^{N} h_x(\sigma_x^{(3)} - 1) \tag{1.1}$$

where $\sigma_x^{(1)}, \sigma_x^{(2)}, \sigma_x^{(3)}$ are Pauli matrices. We denote the wavefunctions $\Phi(s_0, \dots, s_N)$ where s_k is the projection of the spin of the electron on the k^{th} site and can take values up or down.

In the equivalent particle representation, up spins are identified with sites where a particle is present and down spins with empty sites. Since the particle number is conserved, it is legitimate to restrict to sectors with a fixed number of particles $M \geq 0$ and write wavefunctions in that sector as $\Psi(x_1, \dots, x_M)$. In second quantization notations, the Hamiltonian operator in the M particle sector can be written as follows:

$$\mathbb{H} = \sum_{x=0}^{N-1} J_x(a_x^\dagger a_{x+1} + a_{x+1}^\dagger a_x) + \sum_{x=0}^{N} h_x a_x^\dagger a_x, \tag{1.2}$$

where a_x, $a_x^\dagger$ are the creation and annihilation operators for lattice Bosons with hard-core repulsion.

Let R be the reflection operator acting as follows in the Bose-Fock sector with fixed number M of particles:

$$R\Phi(s_0, \dots, s_N) = \Phi(s_N, \dots, s_0) \tag{1.3}$$

in the spin representation and

$$R\Psi(x_0, \dots, x_M) = \Psi(N - x_0, \dots, N - x_M) \tag{1.4}$$

in the particle representation. The operator $\mathbb{H}$ is called *mirror periodic of period* ω in case

$$e^{i\omega\mathbb{H}} = R. \tag{1.5}$$

In [1], the authors give two examples of mirror periodic quantum spin chains whose eigenfunctions can be expressed in analytically closed form in terms of hypergeometric polynomials

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in the discrete Askey-Wilson series [2], namely the Krawtchouk and Hahn polynomials [5]. In [4], it was noticed that more general quantum spin chains can be constructed by numerically solving an inverse spectral theorem. This method is however limited to short chains by practical considerations. In [7], the Hamiltonian for the system is determined after freely choosing the eigenvalue spectrum. The spectrum is thus more general than linear or quadratic, but the eigenfunctions are not known in closed form.

In this article, we solve instead the problem of classifying all possible generalizations of the quantum spin chain in [1] such that the eigenfunctions can be computed in analytically closed form by means of hypergeometric polynomials. We extend the known solutions to eigenfunctions built upon the Racah polynomials, the most general polynomials of the Askey scheme, and find explicit conditions on the eigenvalues for the dynamics to be mirror-periodic. We also demonstrate how the solution in [1] is recovered within this scheme and how the result can be extended to the case of zero lattice spacing for the spin chain, i.e. to the continuous limit.

The paper is organized as follows. In Section 2, we recall the proof of the necessary and sufficient conditions on the eigenfunctions and corresponding eigenvalues for the dynamics to enjoy the mirror-periodicity property. We then prove the main classification result which states the conditions under which a mirror-periodic Hamiltonian has quadratic eigenvalues with corresponding eigenfunctions expressed in terms of the Racah polynomials. We then show how to recover the results obtained in [1]. The Hahn quantum spin chain is treated in Section 3 and the Krawtchouk quantum spin chain in Section 4. Section 5 contains the continuous limits, for which the eigenfunctions are expressed in terms of the Gegenbauer (or ultraspherical) polynomials, the Chebyshev polynomials and the Hermite polynomials respectively.

2. Mirror-periodic Racah quantum spin chains

The construction is based on the following result established in [1], for which we recall the proof.

Theorem 2.1. *The ground state energy of $\mathbb{H}$ is zero in the one particle sector. The eigenvalues of $\mathbb{H}$ in the M particle sector are given by*

$$E_{n_1,\dots,n_M} = \sum_{i=1}^{M} E_{n_i} \tag{2.1}$$

for all sequences $0 \leq n_1 < \ldots < n_M \leq N$. The corresponding eigenfunction $\Psi(x_1,\dots,x_M)$ in the particle representation is given by the Slater determinant:

$$\Psi(x_1,\dots,x_M) = \frac{1}{\sqrt{M!}} \begin{vmatrix} \psi_{n_1}(x_1) & \cdots & \psi_{n_1}(x_M) \\ \vdots & \ddots & \vdots \\ \psi_{n_M}(x_1) & \cdots & \psi_{n_M}(x_M) \end{vmatrix} \tag{2.2}$$

in the sector $x_1 < \ldots < x_M$, while for more general values of the arguments $(x_1,\dots,x_M)$, the wavefunction $\Psi(x_1,\dots,x_M)$ can be obtained by symmetrization.

The Hamiltonian $\mathbb{H}$ is mirror periodic of period $\omega = q\pi$ ($q \in \mathbb{Z}$) if and only if the eigenfunctions $\psi_n(x)$ and corresponding eigenvalues λ_n of the single particle Hamiltonian $\mathbb{H}_1$, which solve

$$\mathbb{H}_1\psi_n(x) = \lambda_n\psi_n(x), \tag{2.3}$$

have the following two properties for all $n, x = 0,\dots,N$:

(i) $\lambda_n = \frac{n}{q} \mod \frac{2}{q}$,
(ii) $\psi_n(N-x) = (-1)^n\psi_n(x)$.

Proof. The proof proceeds in two steps: we first focus on the one particle sector and then extend the result to all other sectors by using Fermionization techniques similar to those introduced by Lieb and Wu in [6].

The one-particle Hamiltonian $\mathbb{H}_1$ is defined on the Hilbert space $l^2(\Lambda_N)$, with $\Lambda_N = \{0, 1, \ldots, N\}$, supported on the chain of $N + 1$ sites labeled by $x \in \Lambda_N$ and has the form

$$\mathbb{H}_1\psi(x) = J_x\psi(x + 1) + J_{x-1}\psi(x - 1) + h_x\psi(x). \tag{2.4}$$

We first show that the Hamiltonian $\mathbb{H}_1$ is mirror periodic of period $\omega = 4\pi$ if and only if its eigenfunctions $\psi_n(x)$ and corresponding eigenvalues λ_n satisfy conditions (i) and (ii) of the theorem. Let $\phi_0(x) \in l^2(\Lambda_N)$ be any initial condition. $\phi_0(x)$ can be expanded as follows:

$$\phi_0(x) = \sum_{n=0}^{N} a_n\psi_n(x). \tag{2.5}$$

Noticing that

$$\phi_0(N - x) = \sum_{n=0}^{N} a_n\psi_n(N - x) = \sum_{n=0}^{N}(-1)^n a_n\psi_n(x) \tag{2.6}$$

and that

$$e^{-iq\pi\lambda_n} = (-1)^n \tag{2.7}$$

proves the following

$$e^{-it\mathbb{H}_1}\phi_0(x) = \phi_0(N - x) \tag{2.8}$$

in case $t = q\pi \mod q2\pi$. The converse follows from the same argument.

The second part of the argument uses the Fermionization technique first introduced by Lieb and Wu in [6]. Consider now the restriction $\mathbb{H}_M$ of the Hamiltonian $\mathbb{H}$ to the sector with M particles. Wavefunctions of $\mathbb{H}_M$ have the form $\Psi(x_1, \ldots, x_M; t)$ and are fully symmetric in the arguments. To find solutions of the dynamical equations it is convenient to consider the function $\Phi(x_1, \ldots, x_M; t)$ which is however completely antisymmetric with respect to all of its arguments and is such that

$$\Phi(x_1, \ldots, x_M; t) = \Psi(x_1, \ldots, x_M; t) \tag{2.9}$$

in case the arguments are ordered so that $x_1 < \ldots < x_M$. The wavefunction Φ describes a system of Fermions with their spins aligned in the same direction, as opposed to the wavefunction Ψ which describes spinless Bosons. One crucial point is that the function $\Phi(x_1, \ldots, x_M; t)$ also satisfies the equations of motion

$$i\frac{\partial}{\partial t}\Phi(x_1, \ldots, x_M; t) = \mathbb{H}_M\Phi(x_1, \ldots, x_M; t). \tag{2.10}$$

This is due to the fact that the Hamiltonian $\mathbb{H}_M$ includes a hard-core repulsion term, so two particles cannot both sit on the same site. Hence, the spectrum on $\mathbb{H}_M$ is the same in the two sectors and the corresponding eigenfunctions are equal in case arguments are ordered, i.e. $x_1 < \ldots < x_M$. The other important remark is that in the Fermion representation the hard core term in $\mathbb{H}_M$ is ineffectual as two electrons cannot both be on the same site due to the Pauli exclusion principle. Hence the spectrum of the Hamiltonian $\mathbb{H}_M$ can be constructed as the sum of the single particle spectra, except that states where one of these states is multiply occupied are forbidden by the exclusion principle. The statement of the theorem follows from these considerations. □

We now define the *Racah quantum spin chain* as the most general quantum spin chain with eigenfunctions expressed using hypergeometric polynomials in the Askey scheme and give a constructive proof for the expression of the normalized eigenfunctions and eigenvalues.

Definition 2.2. The *Racah quantum spin chain* is defined as the quantum spin chain modeled by the Hamiltonian of the form (1.1) with nearest neighbor exchange couplings J_x, $x = 0, \ldots, N-1$ specified as follows:

$$J_x = \frac{B(x)}{|B(x)|}\sqrt{B(x)D(x + 1)} \tag{2.11}$$

and the Zeeman term given by

$$h_x = -B(x) - D(x) \tag{2.12}$$

with $B(x)$ and $D(x)$ directly related to the Racah polynomials and defined as

$$\begin{aligned} B(x) &= 4\,\frac{(x+\alpha+1)(x+\beta+\delta+1)(x-N-\delta)(x-N)}{(2x-N)(2x+1-N)}, \\ D(x) &= 4\,\frac{x(x-\alpha-N-1)(x-\beta-\delta-N-1)(x+\delta)}{(2x-N-1)(2x-N)}. \end{aligned} \tag{2.13}$$

Mirror symmetry implies the following conditions on the Hamiltonian:

$$J_x = J_{N-x-1} \quad \text{and} \quad h_x = h_{N-x}. \tag{2.14}$$

In the case of the Racah chain, the latter is satisfied if and only if the relation

$$\gamma + \delta + 1 = -N \tag{2.15}$$

holds for the functions $B(x)$ and $D(x)$ defined by (A.6) in their generality. Furthermore, for the Hamiltonian to be well defined for all $x \in \Lambda_N$, we need one extra condition in the following table:

1. N even	2. N odd
$\alpha + 1 = -N/2$	$\alpha + 1 = -\frac{N-1}{2}$
$\beta + \delta + 1 = -N/2$	$\beta + \delta + 1 = -\frac{N-1}{2}$
$\delta = -N/2$	$\delta = -\frac{N+1}{2}$

This last condition sets the choice of family for the Racah polynomials on a half-chain. The three solutions for N even in the left column are equivalent, since all cases yield the same Hamiltonian with only two independent parameters. The same remark holds for the right column, N odd. The case N even is however to be distinguished from the case N odd.

2.1. **Racah chain with an odd number of sites (N even).** Without loss of generality for N even, we take $\delta = -N/2$. The Hamiltonian is then defined through:

$$\begin{aligned} B(x) &= 2\,\frac{(x-N)(x+\alpha+1)(x+\beta+1-N/2)}{(2x-N+1)} \\ D(x) &= 2\,\frac{x(x-\alpha-N-1)(x-\beta-1-N/2)}{(2x-N-1)}. \end{aligned} \tag{2.16}$$

Some obvious conditions must be placed on α, β such that the J_x remain real for all $x \in \Lambda_N$:

$$\left\{ \begin{array}{l} \alpha \in \mathbb{R} \setminus [-N,-1] \\ \beta \in (-1,0) \end{array} \right. \quad \text{or} \quad \left\{ \begin{array}{l} \alpha \in (-\frac{N}{2}-1, -\frac{N}{2}) \\ \beta \in \mathbb{R} \setminus [-\frac{N}{2}, \frac{N}{2}-1]. \end{array} \right. \tag{2.17}$$

The two sets of conditions are equivalent under a shift in the parameters α and β by $\pm\frac{N}{2}$ respectively. So we only require the set of conditions on the left. We then solve the eigenvalue equation for the single-particle Hamiltonian to obtain the following:

(1) For $n \le N/2$, we get all the mirror symmetric solutions:

$$\psi_n(x) = \frac{1}{d_n}\,\sqrt{w(x)}\;R_n(\lambda(x)). \tag{2.18}$$

$R_n(\lambda(x))$ are the Racah polynomials (defined by (A.1)) on the half-lattice $x \in [0, \ldots, N/2]$ which extend by mirror symmetry to the whole lattice Λ_N:

$$R_n(\lambda(x)) = {}_4F_3\left(\begin{array}{c} -n, n+\alpha+\beta+1, -x, x-N \\ \alpha+1, \beta+1-N/2, -N/2 \end{array} \middle|\, 1 \right).$$

The weight, given by (A.3), reduces to

$$w(x) = \frac{(\alpha+1)_x(\beta+1-N/2)_x(-N)_x}{(-\alpha-N)_x(-\beta-N/2)_x x!} \tag{2.19}$$

and the normalization factor is

$$d_n^2 = 2\ M\ \frac{(n+\alpha+\beta+1)_n(\alpha+\beta+N/2+2)_n(\alpha+N/2+1)_n(\beta+1)_n n!}{(\alpha+\beta+2)_{2n}(\alpha+1)_n(\beta-N/2+1)_n(-N/2)_n}$$

with

$$M = \frac{(\alpha+\beta+2)_{N/2}(N/2)_{N/2}}{(\alpha+N/2+1)_{N/2}(\beta+1)_{N/2}}.$$

The corresponding eigenvalue is

$$\lambda_n = 2n(2n+2\alpha+2\beta+2). \tag{2.20}$$

(2) For $n > N/2$, we get all the mirror anti-symmetric solutions which are not given in terms of Racah polynomials but are still ${}_4F_3$ hypergeometric functions, which we write as follows:

$$\psi_n(x) = \frac{1}{d_n}\ \sqrt{w(x)}\ R_{N-n-\beta}(\lambda(x))\ \left(1_{\{x\le N/2\}} - 1_{\{x>N/2\}}\right) \tag{2.21}$$

where

$$R_{N-n-\beta}(\lambda(x)) = {}_4F_3\left(\begin{matrix}\beta+n-N, N-n+\alpha+1, -x, x-N\\ \alpha+1, \beta+1-N/2, -N/2\end{matrix}\ \middle|\ 1\right)$$

and the weight remains the same as (2.19), with corresponding eigenvalue

$$\lambda_n = \big(2(N-n)+1-(2\beta+1)\big)\big(2(N-n)+1+2\alpha+1\big). \tag{2.22}$$

The normalization factor is

$$d_n^2 = 2\ M\ \frac{(N-n+\alpha-\beta+1)_{N-n}(\alpha-\beta+N/2+1)_{N-n}(\alpha+N/2+2)_{N-n}}{(\alpha-\beta+2)_{2(N-n)}(\alpha+1)_{N-n}(-\beta-N/2)_{N-n}(1-N/2)_{N-n}} \cdot (1-\beta)_{N-n}(N-n)!$$

with

$$M = \frac{(\alpha-\beta+2)_{N/2-1}(N/2+1)_{N/2-1}}{(\alpha+N/2+2)_{N/2-1}(1-\beta)_{N/2-1}}.$$

2.2. **Racah chain with an even number of sites (N odd).** The solution for N odd is obtained in a similar way. Once again, without loss of generality, we choose the condition $\delta = -\frac{N+1}{2}$. The Hamiltonian is then well defined through:

$$\begin{aligned} B(x) &= 2\ \frac{(x-N)(x+\alpha+1)(x+\beta-N/2+1/2)}{(2x-N)}, \\ D(x) &= 2\ \frac{x(x-\alpha-N-1)(x-\beta-N/2-1/2)}{(2x-N)}. \end{aligned} \tag{2.23}$$

α, β are moreover conditioned to J_x being real for all $x \in \Lambda_N$. The sets of conditions on α and β are either

$$\begin{cases} \alpha \in \mathbb{R}\setminus[-N,-1] \\ \beta \in (-1,1) \end{cases} \quad \text{or} \quad \begin{cases} \alpha \in (\frac{N-3}{2}, \frac{N+1}{2}) \\ \beta \in \mathbb{R}\setminus[-\frac{N-1}{2}, \frac{N-1}{2}] \end{cases} \tag{2.24}$$

which are equivalent under a shift in the parameters. So we only require the one on the left. We then solve the eigenvalue equation for the Hamiltonian operator.

(1) for $n \le \frac{N-1}{2}$, we get all the mirror symmetric solutions:

$$\psi_n(x) = \frac{1}{d_n}\ \sqrt{w(x)}\ R_n(\lambda(x)) \tag{2.25}$$

where the Racah polynomials are

$$R_n(\lambda(x)) = {}_4F_3\left(\begin{matrix}-n, n+\alpha+\beta+1, -x, x-N\\ \alpha+1, \beta+1/2-N/2, 1/2-N/2\end{matrix}\ \middle|\ 1\right),$$

the weight is given by

$$w(x) = \frac{(\alpha+1)_x(\beta+1/2-N/2)_x(-N)_x(1-N/2)_x}{(-\alpha-N)_x(-\beta+1/2-N/2)_x x!(-N/2)_x} \tag{2.26}$$

and the normalization factor is

$$d_n^2 = 2\ M\ \frac{(n+\alpha+\beta+1)_n(\alpha+\beta+N/2+3/2)_n(\alpha+N/2+3/2)_n(\beta+1)_n n!}{(\alpha+\beta+2)_{2n}(\alpha+1)_n(\beta-N/2+1/2)_n(-N/2+1/2)_n}$$

with

$$M = \frac{(\alpha+\beta+2)_{\frac{N-1}{2}}(N/2+1/2)_{\frac{N-1}{2}}}{(\alpha+N/2+3/2)_{\frac{N-1}{2}}(\beta+1)_{\frac{N-1}{2}}}.$$

The corresponding eigenvalue is

$$\lambda_n = 2n(2n+2\alpha+2\beta+2). \tag{2.27}$$

(2) for $n \geq \frac{N+1}{2}$, we get all the mirror anti-symmetric solutions which are given in terms ${}_4F_3$ hypergeometric functions:

$$\psi_n(x) = \frac{1}{d_n}\ \sqrt{w(x)}\ R_{N-n-\beta}(\lambda(x))\ \left(1_{\{x<N/2\}} - 1_{\{x>N/2\}}\right) \tag{2.28}$$

where

$$R_{N-n-\beta}(\lambda(x)) = {}_4F_3\left(\begin{matrix}\beta+n-N, N-n+\alpha+1, -x, x-N \\ \alpha+1, \beta+1/2-N/2, 1/2-N/2\end{matrix}\ \middle|\ 1\right).$$

The weight remains the same as (2.26), but the normalization factor is slightly different,

$$\begin{aligned} d_n^2 \quad &= \quad 2\ M\ \frac{(N-n+\alpha-\beta+1)_{N-n}(\alpha-\beta+\frac{N+3}{2})_{N-n}(\alpha+\frac{N+3}{2})_{N-n}}{(\alpha-\beta+2)_{2(N-n)}(\alpha+1)_{N-n}(\frac{1-N}{2}-\beta)_{N-n}(\frac{1-N}{2})_{N-n}} \\ &\quad \cdot (1-\beta)_{N-n}(N-n)! \end{aligned}$$

with

$$M = \frac{(\alpha-\beta+2)_{\frac{N-1}{2}}(N/2+1/2)_{\frac{N-1}{2}}}{(\alpha+N/2+3/2)_{\frac{N-1}{2}}(1-\beta)_{\frac{N-1}{2}}}.$$

The corresponding eigenvalue is given by

$$\lambda_n = \big(2(N-n)+1-(2\beta+1)\big)\big(2(N-n)+1+2\alpha+1\big).$$

For N both even and odd, we conclude that the mirror symmetry property, $\psi_n(x) = \psi_n(N-x)$, in case $n \leq N/2$, is easily verified since

$$R_n(\lambda(x)) = R_n(\lambda(N-x)) \quad \text{and} \quad w(x) = w(N-x). \tag{2.29}$$

In case $n > N/2$, the same reasoning with

$$R_{N-n-\beta}(\lambda(x)) = R_{N-n-\beta}(\lambda(N-x)) \quad \text{and} \quad w(x) = w(N-x) \tag{2.30}$$

yields the mirror anti-symmetry property: $\psi_n(x) = -\psi_n(N-x)$.

The latter result hence gives condition (ii) in Theorem 2.1. It remains to show that condition (i) holds as well. That is, for a period $\omega = q\pi$ ($q \in \mathbb{Z}$), the propagator offsets the phase acquired by mirror-periodicity. The two cases for N even and odd can be treated simultaneously. We first recast the symmetric and anti-symmetric eigenvalues into

$$\lambda_k = \begin{cases} k(k+2\alpha+2\beta+2) & \text{if } k \in 2\mathbb{Z} \\ \big(k-(2\beta+1)\big)(k+2\alpha+1) & \text{if } k \in 2\mathbb{Z}+1. \end{cases} \tag{2.31}$$

To offset the phase, Theorem 2.1 requires

$$e^{-i\omega\lambda_k} = (-1)^k, \tag{2.32}$$

which leads to the following conditions on α, β:

- for k even, $e^{-iq\pi\lambda_k} = 1$ implies:

$$2q(\alpha+\beta) \in \mathbb{Z}. \tag{2.33}$$

- for k odd, $e^{-iq\pi\lambda_k} = -1$ implies:

$$2q(k+1)(\alpha-\beta) - 4q\alpha(\beta+1) \in 2\mathbb{Z}+1. \tag{2.34}$$

The second condition yields

$$4q\alpha(\beta+1) \in 2\mathbb{Z}+1 \tag{2.35}$$

since $k+1$ is even. When combining it to the first one, we get

$$4q\beta(\alpha-1) \in 2\mathbb{Z}+1. \tag{2.36}$$

The two requirements thus imply the following general form for the parameters α and β:

$$\alpha = \frac{2p_1+1}{2q_1} \qquad \beta = \frac{2p_2+1}{2q_2} \tag{2.37}$$

where $p_1, p_2, q_1, q_2 \in \mathbb{Z}$ with $q_1 q_2 = q$.

3. Mirror-periodic Hahn quantum spin chains

The result on the Hahn quantum spin chain derived in [1] is easily recovered from the Racah quantum spin chain.

Definition 3.1. The *Hahn quantum spin chain* is defined as the quantum spin chain modeled by the Hamiltonian of the form (1.1) with nearest neighbor exchange couplings J_x, $x = 0, \ldots, N-1$ specified as follows:

$$J_x = \sqrt{(x+\alpha+1)(x-N)(x+1)(x-\alpha-N)} \tag{3.1}$$

and the Zeeman term given by

$$h_x = -(x+\alpha+1)(x-N) - x(x-\alpha-N-1). \tag{3.2}$$

Proposition 3.1. *The Hahn quantum spin chain is recovered from the Racah quantum spin chain by setting $\beta = -\frac{1}{2}$. Moreover, it satisfies the mirror-periodicity property of period $\omega = q\pi$ if and only if $\alpha = \dfrac{2p+1}{2q}$ with $p \in \mathbb{Z}$.*

Proof. Setting $\beta = -\frac{1}{2}$ in equivalently (2.16) or (2.23) yields the Hamiltonian in Definition 3.1. The solutions to the eigenvalue equation for the single-particle Hamiltonian are

$$\psi_k(x) = \frac{1}{d_k}\,\sqrt{w(x)}\;Q_k(x;\alpha,\alpha,N) \tag{3.3}$$

for $k = 0, \ldots, N$ and with

$$Q_k(x;\alpha,\alpha,N) = {}_3F_2\left(\begin{matrix} -k, k+2\alpha+1, -x \\ \alpha+1, -N \end{matrix}\,\middle|\, 1\right).$$

The weight is given by

$$w(x) = \binom{\alpha+x}{x}\binom{\alpha+N-x}{N-x}$$

and the normalization factor is

$$d_k^2 = \frac{(-1)^k (k+2\alpha+1)_{N+1} k!}{(2k+2\alpha+1)(-N)_k N!}.$$

Clearly, we have $w(N-x) = w(x)$. Now consider the generating function relation

$${}_1F_1\left(\begin{matrix} -x \\ \alpha+1 \end{matrix}\,\middle|\, -t\right) {}_1F_1\left(\begin{matrix} x-N \\ \alpha+1 \end{matrix}\,\middle|\, t\right) = \sum_{k=0}^{N} \frac{(-N)_k}{(\alpha+1)_k k!} Q_k(x;\alpha,\alpha,N) t^k \tag{3.4}$$

from which we deduce

$$\sum_{k=0}^{N} \frac{(-N)_k}{(\alpha+1)_k k!} Q_k(N-x;\alpha,\alpha,N)(-t)^k = \sum_{k=0}^{N} \frac{(-N)_k}{(\alpha+1)_k k!} Q_k(x;\alpha,\alpha,N) t^k. \tag{3.5}$$

It follows that

$$Q_k(x;\alpha,\alpha,N) = (-1)^k Q_k(N-x;\alpha,\alpha,N). \tag{3.6}$$

So $\psi_k(x)$ is either reflection symmetric or anti-symmetric. The corresponding eigenvalue is

$$\lambda_k = k(k+2\alpha+1).$$

Conditions (2.37) imply $\alpha = \dfrac{2p+1}{2q}$, where p is an integer, such that $e^{-iq\pi\lambda_k} = (-1)^k$. □

4. Mirror-periodic Krawtchouk quantum spin chains

The mirror-periodicity property in the Krawtchouk quantum spin chain was already discovered in [1]. In an even earlier work, Atakishiev et al. [3] used the Krawtchouk polynomials as a basis for quantum chains admitting periodic solutions. We show how the mirror-periodicity result fits into the classification framework.

Definition 4.1. The *Krawtchouk quantum spin chain* is defined as the quantum spin chain modeled by the Hamiltonian of the form (1.1) with nearest neighbor exchange couplings J_x, $x = 0,\ldots,N-1$ specified as follows:

$$J_x = \frac{1}{2}\sqrt{(N-x)(x+1)} \tag{4.1}$$

and the Zeeman term given by

$$h_x = \frac{N}{2}. \tag{4.2}$$

Proposition 4.1. *The Krawtchouk quantum spin chain is recovered from the Racah quantum spin chain by setting $\beta = -\frac{1}{2}$ and taking the limit $\alpha \to \infty$. Moreover, it satisfies the mirror-periodicity property of period $\omega = \pi$.*

Proof. Once rescaled by $\frac{1}{2\alpha}$, the Hahn Hamiltonian converges in the limit $\alpha \to \infty$ to the Krawtchouk Hamiltonian in Definition 4.1. The solutions to the eigenvalue equation for the single-particle Hamiltonian converge to

$$\psi_k(x) = \frac{1}{d_k}\,\sqrt{w(x)}\;K_k\left(x;\frac{1}{2},N\right) \tag{4.3}$$

for $k = 0,\ldots,N$ and with

$$K_k\left(x;\frac{1}{2},N\right) = {}_2F_1\left(\left.\begin{matrix}-k,-x\\-N\end{matrix}\,\right|\,2\right).$$

The ratio of the weight and normalization factor converges to

$$w(x) = \frac{1}{2^N}\,\frac{N!}{\Gamma(x+1)\Gamma(N-x+1)} \quad \text{over} \quad d_k^2 = \frac{(-1)^k k!}{(-N)_k}.$$

The reflection symmetry $w(N-x) = w(x)$ is obvious. In the limit $\alpha \to \infty$, (3.6) converges to

$$K_k\left(x;\frac{1}{2},N\right) = (-1)^k K_k\left(N-x;\frac{1}{2},N\right). \tag{4.4}$$

So $\psi_k(x)$ is either reflection symmetric or anti-symmetric. The corresponding eigenvalue, once divided by 2α, converges to

$$\lambda_k = k,$$

which implies $e^{-i\omega k} = (-1)^k$ if and only if the period $\omega = \pi \mod 2\pi$. □

5. Mirror-periodicity in the continuous limit

Discrete orthogonal polynomials of the Askey scheme converge to continuous orthogonal polynomials under specific limit relations described in the Askey scheme [5]. We investigate the consequence of these relations on the mirror-periodicity property.

5.1. **The Gegenbauer or ultraspherical continuous limit.**

Definition 5.1. The Gegenbauer or ultraspherical polynomials are the Jacobi polynomials restricted to $\alpha = \beta = \lambda - \frac{1}{2}$ $(\lambda \neq 0)$ and with another normalization:

$$C_k^{(\lambda)}(z) = \frac{(2\lambda)_k}{k!} \; {}_2F_1\left(\begin{matrix} -k, k+2\lambda \\ \lambda + \frac{1}{2} \end{matrix} \,\middle|\, \frac{1-z}{2} \right) \tag{5.1}$$

for $k = 0, 1, 2, \ldots$ and $z \in [-1, 1]$.

The ultraspherical polynomials can be obtained from the Hahn polynomials by rescaling $x \mapsto \frac{N}{2}(1-z)$ before taking the limit $N \to \infty$:

$$\lim_{N\to\infty} Q_k\left(\frac{N}{2}(1-z); \lambda - \frac{1}{2}, \lambda - \frac{1}{2}, N\right) = \frac{C_k^{(\lambda)}(z)}{C_k^{(\lambda)}(1)} \tag{5.2}$$

where $z \in [-1, 1]$.

Proposition 5.1. *The ultraspherical continuous limit is obtained from the Hahn quantum spin chain by rescaling $x \mapsto \frac{N}{2}(1-z)$ before taking the limit $N \to \infty$. It satisfies the mirror-periodicity property of period $\omega = q\pi$ if and only if*

$$\lambda - \frac{1}{2} = \frac{2p+1}{2q} \tag{5.3}$$

where p is an integer.

Proof. The Hamiltonian has the continuous limit on $[-1, 1]$:

$$\mathbb{H} = (1 - z^2)\frac{\partial^2}{\partial z^2} - (2\lambda + 1) z \frac{\partial}{\partial z} \tag{5.4}$$

and satisfies a reflection symmetry condition with respect to $z = 0$. The solutions to the eigenvalue equation are

$$\psi_k(z) = \frac{1}{d_k} \sqrt{\rho(z)}\; C_k^{(\lambda)}(z) \tag{5.5}$$

where

$$\rho(z) = (1 - z^2)^{\lambda - \frac{1}{2}}$$

and

$$d_k^2 = \frac{\pi\, \Gamma(k + 2\lambda) 2^{1-2\lambda}}{\{\Gamma(\lambda)\}^2 (k + \lambda) k!}.$$

The invariant measure is symmetric about the axis $z = 0$: $\rho(-z) = \rho(z)$. The generating function, given by

$$(1 - 2zt + t^2)^{-\lambda} = \sum_{k=0}^{\infty} C_k^{(\lambda)}(z) t^k, \tag{5.6}$$

implies

$$C_k^{(\lambda)}(z) = (-1)^k C_k^{(\lambda)}(-z). \tag{5.7}$$

So the solution $\psi_k(z)$ is either symmetric or anti-symmetric about the axis $z = 0$. The corresponding eigenvalue is

$$\lambda_k = k(k + 2\lambda). \tag{5.8}$$

Condition (5.3) is then straightforward from Proposition 3.1. □

Remark 5.2. The Jacobi polynomials are the most general hypergeometric polynomials orthogonal with respect to a measure with support on the real line. The Racah polynomials do not have a continuous limit, whereas the Hahn polynomials converge to the Jacobi polynomials. The restrictions on α in the Hahn case imply that the ultraspherical continuous limit gives the most general solvable mirror-periodic continuous solutions.

5.2. **The Chebyshev continuous limit.**

Definition 5.3. The Chebyshev polynomials of the first kind are the ultraspherical polynomials in the case $\lambda = 0$ and with another normalization:

$$T_k(z) = {}_2F_1\left(\begin{matrix}-k, k \\ \frac{1}{2}\end{matrix} \middle| \frac{1-z}{2}\right) \tag{5.9}$$

for $k = 0, 1, \ldots$ and $z \in [-1, 1]$.

Proposition 5.2. *The Chebyshev continuous limit is obtained from the ultraspherical continuous limit in the case $\lambda = 0$. It satisfies the mirror-periodicity property of period $\omega = \pi$.*

Proof. The Hamiltonian operator on $[-1, 1]$, given by

$$\mathbb{H} = (1 - z^2)\frac{\partial^2}{\partial z^2} - z\frac{\partial}{\partial z}, \tag{5.10}$$

satisfies a reflection symmetry condition with respect to $z = 0$. The solutions to the eigenvalue equation are

$$\psi_k(z) = \frac{1}{d_k}\ \sqrt{\rho(z)}\ T_k(z) \tag{5.11}$$

where the invariant measure is $\rho(z) = (1 - z^2)^{-1}$ and the normalization factors $d_k^2 = \frac{\pi}{2}$ for $k = 1, 2, \ldots$ and $d_0^2 = \pi$. The invariant measure is symmetric about the axis $z = 0$: $\rho(-z) = \rho(z)$. The generating function, given by

$$\frac{1 - zt}{1 - 2zt + t^2} = \sum_{k=0}^{\infty} T_k(z)t^k, \tag{5.12}$$

implies

$$T_k(z) = (-1)^k T_k(-z). \tag{5.13}$$

So the solution $\psi_k(z)$ is either symmetric or anti-symmetric about the axis $z = 0$. The corresponding eigenvalue,

$$\lambda_k = k^2, \tag{5.14}$$

implies mirror-periodicity of period $\omega = \pi$. □

5.3. **The Hermite (or harmonic oscillator) continuous limit.**

Definition 5.4. The Hermite polynomials are defined as follows:

$$H_k(z) = (2z)^k {}_2F_0\left(\begin{matrix}-\frac{k}{2}, -\frac{k-1}{2} \\ -\end{matrix} \middle| -\frac{1}{z^2}\right) \tag{5.15}$$

for $k = 0, 1, \ldots$ and $z \in \mathbb{R}$.

The Hermite polynomials can be obtained from the ultraspherical polynomials by taking $\alpha = \lambda - \frac{1}{2}$ and letting $\alpha \to \infty$ as follows:

$$\lim_{\alpha\to\infty} \alpha^{-\frac{k}{2}} C_k^{(\alpha+\frac{1}{2})}\left(\frac{z}{\sqrt{\alpha}}\right) = \frac{1}{k!}\ H_k(z). \tag{5.16}$$

Proposition 5.3. *The Hermite continuous limit is obtained from the ultraspherical continuous limit by rescaling $z \mapsto \frac{z}{\sqrt{\alpha}}$, for $\alpha = \lambda - \frac{1}{2}$, before taking the limit $\alpha \to \infty$. It satisfies the mirror-periodicity property of period $\omega = \pi$.*

Proof. The Hamiltonian rescaled by $\frac{1}{2}$ has the following continuous limit on $\mathbb{R}$:

$$\mathbb{H} = \frac{1}{2}\frac{\partial^2}{\partial z^2} - z\frac{\partial}{\partial z} \tag{5.17}$$

and satisfies a reflection symmetry condition with respect to $z = 0$. The solutions to the eigenvalue equation are the normalized Hermite functions

$$\psi_k(z) = \frac{1}{\sqrt{2^k k! \sqrt{\pi}}}\; e^{-\frac{z^2}{2}}\; H_k(z). \tag{5.18}$$

$\psi_k(z)$ is either symmetric or anti-symmetric about the axis $z = 0$. The corresponding eigenvalue is

$$\lambda_k = k, \tag{5.19}$$

which implies mirror-periodicity of period $\omega = \pi$. □

Remark 5.5. The Hermite continuous limit can also be obtained from the Krawtchouk quantum spin chain as the Hermite polynomials satisfy the following limit relation:

$$\lim_{N\to\infty} \sqrt{\binom{N}{k}} K_k\left(\frac{N}{2} + \sqrt{\frac{N}{2}}z; \frac{1}{2}, N\right) = \frac{(-1)^k}{\sqrt{2^k k!}}\; H_n(z) \tag{5.20}$$

where $z \in \mathbb{R}$.

Remark 5.6. The latter Hamiltonian is related to the harmonic oscillator Hamiltonian through the gauge transformation $g(z) = \exp\left(\frac{z^2}{2}\right)$:

$$g^{-1}\mathbb{H}\; g = \frac{1}{2}\frac{\partial^2}{\partial z^2} + \frac{1}{2}(1 - z^2). \tag{5.21}$$

Appendix A. Definitions and properties of the Racah polynomials

Definition A.1. The Racah polynomials $R_n(\lambda(x)) := R_n(\lambda(x); \alpha, \beta, \gamma, \delta)$ are defined as follows:

$$R_n(\lambda(x); \alpha, \beta, \gamma, \delta) = {}_4F_3\left(\begin{matrix} -n, n+\alpha+\beta+1, -x, x+\gamma+\delta+1 \\ \alpha+1, \beta+\delta+1, \gamma+1 \end{matrix} \;\middle|\; 1\right) \tag{A.1}$$

where ${}_4F_3$ is a hypergeometric function, $\lambda(x) = x(x+\gamma+\delta+1)$, $n = 0, 1, 2, \ldots, N$ and x belongs to the lattice $\Lambda_N = \{0, 1, 2, \ldots, N\}$. The Racah polynomials are moreover conditioned to belonging to one of the three families:

1. $\alpha + 1 = -N$,
2. $\beta + \delta + 1 = -N$,
3. $\gamma + 1 = -N$.

The Racah polynomials satisfy an orthogonality relation with respect to a discrete measure supported on the set Λ_N. Namely,

$$\sum_{x\in\Lambda_N} R_m(\lambda(x))R_n(\lambda(x))w(x) = d_n^2 \delta_{nm} \tag{A.2}$$

where the weight $w(x) := w(x; \alpha, \beta, \gamma, \delta)$ is given by

$$w(x) = \frac{(\alpha+1)_x(\beta+\delta+1)_x(\gamma+1)_x(\gamma+\delta+1)_x((\gamma+\delta+3)/2)_x}{(-\alpha+\gamma+\delta+1)_x(-\beta+\gamma+1)_x((\gamma+\delta+1)/2)_x(\delta+1)_x x!} \tag{A.3}$$

and the normalization factor is

$$d_n^2 = M\; \frac{(n+\alpha+\beta+1)_n(\alpha+\beta-\gamma+1)_n(\alpha-\delta+1)_n(\beta+1)_n n!}{(\alpha+\beta+2)_{2n}(\alpha+1)_n(\beta+\delta+1)_n(\gamma+1)_n} \tag{A.4}$$

with

$$M = \begin{cases} \dfrac{(-\beta)_N(\gamma+\delta+2)_N}{(-\beta+\gamma+1)_N(\delta+1)_N} & \text{if } \alpha = -N-1 \\ \dfrac{(-\alpha+\delta)_N(\gamma+\delta+2)_N}{(-\alpha+\gamma+\delta+1)_N(\delta+1)_N} & \text{if } \beta+\delta = -N-1 \\ \dfrac{(\alpha+\beta+2)_N(-\delta)_N}{(\alpha-\delta+1)_N(\beta+1)_N} & \text{if } \gamma = -N-1. \end{cases}$$

The Racah polynomials are solutions to the difference equation

$$B(x)R_n(\lambda(x+1)) - \big(B(x)+D(x)\big)R_n(\lambda(x)) + D(x)R_n(\lambda(x-1)) = \lambda_n R_n(\lambda(x)) \tag{A.5}$$

given by the functions

$$\begin{aligned} B(x) &= 4\,\frac{(x+\alpha+1)(x+\beta+\delta+1)(x+\gamma+1)(x+\gamma+\delta+1)}{(2x+\gamma+\delta+1)(2x+\gamma+\delta+2)}, \\ D(x) &= 4\,\frac{x(x-\alpha+\gamma+\delta)(x-\beta+\gamma)(x+\delta)}{(2x+\gamma+\delta)(2x+\gamma+\delta+1)}, \end{aligned} \tag{A.6}$$

and eigenvalues $\lambda_n = 2n(2n+2\alpha+2\beta+2)$.

References

[1] C. Albanese, M. Christandl, N. Datta, and A. Ekert. Mirror inversion of quantum states in linear registers. *Phys. Rev. Lett.*, 93:230502, 2004.

[2] R. Askey and J. Wilson. A set of orthogonal polynomials that generalized the racah coefficients or 6-j symbols. *SIAM Journal of Mathematical Analysis*, 10:1008–1020, 1979.

[3] N.A. Atakishiev, E.I. Jafarov, S.M. Nagiyev, and K. Wolf. Meixner oscillators. *Rev. Mex. Fis.*, 44:235–44, 1998.

[4] P. Karbach and J. Stolze. Comment on "Mirror inversion of quantum states in linear register". *available at* http://arxiv.org/abs/quant-ph/0501007, 2005.

[5] R. Koekoek and R. Swarttouw. The Askey scheme of hypergeometric orthogonal polynomials and its q-analogue. *Tech. report 98-17, Department of Technical Mathematics and Informatics, Delft University of Technology, Delft, The Netherlands*, 1998.

[6] E. Lieb and F. Wu. Absence of mott transition in an exact solution of the short-range, one-band model in one dimension. *Phys. Rev. Lett.*, 20:1445–1448, 1968.

[7] M.-H. Yung and S. Bose. Perfect state transfer, effective gates and entanglement generation in engineered bosonic and fermionic networks. *available at* http://arxiv.org/abs/quant-ph/0407212, 2004.

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