BOUNDARY EFFECTS IN NON-UNIFORM SPIN CHAINS

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Abstract. We give an explicit comparison of eigenvalues and eigenvectors of XY Hamiltonians of an open linear spin-1/2 chain and a closed spin-1/2 ring with periodic in space coefficients. It is shown that the Hamiltonian of a $k$-periodic chain with $nk - 1$ sites has $(n - 1)k$ multiplicity one eigenvalues which are eigenvalues of multiplicity two for a Hamiltonian of a $k$-periodic ring with $2kn$ sites. For the corresponding eigenvectors in the case of a chain an explicit expression in terms of eigenvectors of the ring Hamiltonian is given. The remaining $k - 1$ eigenvalues of the chain Hamiltonian and $2k$ eigenvalues of the ring Hamiltonian, together with the corresponding eigenvectors, are responsible for the difference between chain and ring models which displays in the boundary effects at the ends of the chain and translation invariance of the periodic ring.

Key Words. exactly soluble spin models, tridiagonal matrices.

1. Introduction

One-dimensional exactly soluble homogeneous spin models (spin chains, rings) serve as a convenient tool for understanding quantum dynamics of spin systems [11]. Over the past few years new exactly solvable examples of non-homogeneous spin systems have been found [4, 9, 10, 12, 16] and this prompts a string of applications to the problems of quantum NMR dynamic [7] and quantum information theory [2, 10, 12]. Another possible direction for the development of the ideas involved in exact solutions for these models would be deeper understanding of spectra and eigenvectors of Hamiltonians of non-homogeneous spin systems with different types of interactions like, for example, Ising model [1]. From this point of view it is important to clarify the difference between open linear spin models and closed ring spin models.

Closed ring models usually posses extra symmetries coming, for example, from translation invariance of the system. Therefore, it is sometimes easier to study such systems through a framework of quantum integrals and reduction of the dimension. Elementary physical arguments show that for a large length a spin ring and a spin chain behave similar at small times and, therefore, one can expect to recognize essential chunk of properties for the chain just by comparing it with the ring. There are also correction terms which become significant when the evolution time is long and we have to take into account those spin wave packets which reflect from the ends of the chain. Though there is no reason to expect these correction terms to be universal and independent from particular properties of the chain, it is still reasonable that their structure reflects merely the difference between the corresponding ring and chain models.
The aim of the present paper is to give a detailed comparison of spectra and eigen-vectors of XY Hamiltonians of an open spin chain and a closed spin ring with periodic in space coefficients. The simplest example is homogeneous XY models which were solved in [3, 14]. It corresponds to the case of period one. It turns out that all eigenvalues for the chain Hamiltonian in homogeneous case have multiplicity one and equal to all but two eigenvalues of a homogeneous spin ring with \(2N + 2\) sites where \(N\) is the length of the open chain. These eigenvalues of the ring Hamiltonian have multiplicity two. Corresponding eigenvectors of the chain Hamiltonian form the first \(N\) components of particularly chosen eigenvectors of the ring Hamiltonian. Due to the extra symmetry these eigenvectors of the ring Hamiltonian can be uniquely reconstructed from the chain eigenvectors. Therefore, the difference of these models is only in properties corresponding to the remaining two eigenvalues of the ring Hamiltonian. We observe the same behavior for every periodic in space chain and ring XY models. In particular, XY Hamiltonian of a \(k\)-periodic spin chain with \(kn - 1\) sites has \(k(n - 1)\) common eigenvalues with XY Hamiltonian of a \(k\)-periodic spin ring with \(2kn\) sites. Remaining eigenvalues of these models are responsible for the reflection of spin wave packets from the ends of the chain and for the translation symmetry of the ring model.

In due course we review some ideas used for the exact solutions of XY models in various settings, which also allows us to see some simplifications comparing to the original proofs. We, thus, present an alternative derivation for the diagonalization of the XY Hamiltonian of an alternating spin chain with odd number of sites, first solved in [9], and for the diagonalization of the XY Hamiltonian of any periodic spin ring, first given in [5].

2. The models

The Hamiltonian of a spin-1/2 open chain with only nearest neighbor (NN) couplings has the following general form

\[
H_{\text{chain}} = \sum_{n=1}^{N} \omega_{n} I_{nz} + \sum_{n=1}^{N-1} D_{n,n+1} (I_{n,x}I_{n+1,x} + I_{n,y}I_{n+1,y}),
\]

where \(\omega_{n} = 1, \ldots, N\), are the Larmor frequencies, and \(D_{n,n+1} \neq 0, n = 1, \ldots, N - 1\), are the NN coupling constants.

The Jordan–Wigner transformation reduces the study of the Hamiltonian (1) to the diagonalization problem of

\[
H_{\text{chain}}^{\text{chain}} = 2\Omega + D_{\text{chain}},
\]

where

\[
\Omega = \begin{bmatrix}
\omega_{1} & 0 & \cdots & 0 & 0 \\
0 & \omega_{2} & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & \omega_{N-1} & 0 \\
0 & 0 & \cdots & 0 & \omega_{N}
\end{bmatrix}, \quad
D_{\text{chain}} = \begin{bmatrix}
0 & D_{1} & \cdots & 0 & 0 \\
D_{1} & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & D_{N-1} \\
0 & 0 & \cdots & D_{N-1} & 0
\end{bmatrix}
\]

\((D_{j} = D_{j,j+1}, j = 1, \ldots, N - 1)\).

Similarly, the Hamiltonian of a spin-1/2 ring with only nearest neighbor couplings has the following general form

\[
H_{\text{ring}} = \sum_{n=1}^{N} \omega_{n} I_{nz} + \sum_{n=1}^{N} D_{n,n+1} (I_{n,x}I_{n+1,x} + I_{n,y}I_{n+1,y}),
\]
where \( \omega_n, n = 1, \ldots, N \), are the Larmor frequencies, \( D_{n,n+1} \neq 0, n = 1, \ldots, N \), are the NN coupling constants, and we assume that spin \( N + 1 \) is the same as spin 1.

The Jordan–Wigner transformation reduces the study of the Hamiltonian (4) to the diagonalization problem of

\[
H^{\text{ring}} = 2\Omega + D^{\text{ring}},
\]

with

\[
\Omega = \begin{bmatrix}
\omega_1 & 0 & \cdots & 0 & 0 \\
0 & \omega_2 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & \omega_{N-1} & 0 \\
0 & 0 & \cdots & 0 & \omega_N
\end{bmatrix}, \\
D^{\text{ring}} = \begin{bmatrix}
0 & D_1 & \cdots & 0 & D_N \\
D_1 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & D_{N-1} \\
D_N & 0 & \cdots & D_{N-1} & 0
\end{bmatrix},
\]

where \( D_j = D_{j,j+1}, j = 1, \ldots, N \), and the matrix \( D^{\text{ring}} \) differs from \( D^{\text{chain}} \) only by the right upper and the left lower corners.

Assume now that the Larmor frequencies and the coupling constants are repeating periodically with a period \( k \), i.e.,

\[
\omega_j = \omega_{j+k}, \quad D_j = D_{j+k}.
\]

In addition to this for the case of the ring model we have to assume that \( N = km \).

We rename the Hamiltonians for the chain and the ring to underline dependence on \( \omega_j, D_j, j = 1, \ldots, k \), and periodicity as

\[
H^{\text{chain}}_N = H^{\text{chain}}_N(\omega_j, D_j, k); \quad H^{\text{ring}}_k = H^{\text{ring}}_k(\omega_j, D_j, k).
\]

In what follows it would be convenient for us to consider independently components of vectors in \( \mathbb{C}^N \) corresponding to different reminders modulo \( k \). We denote these components by \( u_{(j)} \), \( j = 1, 2, \ldots, k \), so that if

\[
u = (u_1, u_2, \ldots, u_N)^t,
\]

then

\[
u_{(j)} = (u_{j}, u_{j+k}, u_{j+2k}, \ldots)^t.
\]

For the ring model all components have exactly \( m \) coordinates, while for the chain with \( km - 1 \) sites the component \( u_{(k)} \) has only \( m - 1 \) coordinates and the other components have exactly \( m \) coordinates. We will also fix a notation

\[
H_{i,j} = \begin{bmatrix}
2\omega_i & D_i & \cdots & 0 & 0 \\
D_i & 2\omega_{i+1} & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 2\omega_{j-1} & D_{j-1} \\
0 & 0 & \cdots & D_{j-1} & 2\omega_j
\end{bmatrix}
\]

for a symmetric three-diagonal \((j - i + 1) \times (j - i + 1)\)-matrix with coefficients \(2\omega_i, \ldots, 2\omega_j, D_i, \ldots, D_{j-1}\). The \( N \times N \) identity matrix will be denoted by \( I_N \).

3. Homogeneous models

We begin our comparison by considering the simplest possible case, i.e. the case of period \( k = 1 \) with equal Larmor frequencies and coupling constants, which is known as a homogeneous model.
Theorem 1. \( H^\text{chain}_N(\omega, D, 1) \) has \( N \) distinct eigenvalues

\[ \lambda_j = 2\omega + 2D \cos \left( \frac{\pi j}{N+1} \right), \quad j = 1, \ldots, N, \]

and the corresponding eigenvectors are of the form

\[ \vec{u}_j = \vec{u}_j(N) = \left( \sin \left( \frac{\pi j}{N+1} \right), \sin \left( \frac{2\pi j}{N+1} \right), \ldots, \sin \left( \frac{N\pi j}{N+1} \right) \right). \]

Similarly,

Theorem 2. \( H^\text{ring}_N(\omega, D, 1) \) has \( N - \lfloor N/2 \rfloor \) distinct eigenvalues

\[ \lambda_j = 2\omega + 2D \cos \left( \frac{2\pi j}{N} \right), \quad 0 \leq j \leq N/2. \]

If \( 0 < j < N/2 \) then \( \lambda_j \) has multiplicity two and the corresponding eigenvectors are of the form

\[ \vec{v}_j = \vec{v}_j(N) = \left( \cos \left( \frac{2\pi j}{N} \right), \cos \left( \frac{2 \cdot 2\pi j}{N} \right), \ldots, \cos \left( \frac{(N-1) \cdot 2\pi j}{N} \right), 1 \right), \]

\[ \vec{w}_j = \vec{w}_j(N) = \left( \sin \left( \frac{2\pi j}{N} \right), \sin \left( \frac{2 \cdot 2\pi j}{N} \right), \ldots, \sin \left( \frac{2 \cdot (N-1)\pi j}{N} \right), 0 \right). \]

If \( j = 0 \) then \( \lambda_j = 2\omega + 2D \) has multiplicity one with an eigenvector

\[ \vec{u} = (1, 1, \ldots, 1). \]

If \( N \) is even and \( j = N/2 \) then \( \lambda_j = 2\omega - 2D \) is an eigenvalue of multiplicity one with an eigenvector

\[ \vec{v} = (1, -1, 1, -1, \ldots, 1, -1). \]

Remark 1. Theorems 1, 2 were obtained in [3, 14]. Proofs of both the theorems are straight forward verifications.

Corollary 1. The spectra of \( H^\text{chain}_N(\omega, D, 1) \) and \( H^\text{ring}_{2N+2}(\omega, D, 1) \) are related to each other by

\[ \det \left( H^\text{chain}_N(\omega, D, 1) - \lambda I_N \right)^2 (2\omega + 2D - \lambda) (2\omega - 2D - \lambda) = \]

\[ \det \left( H^\text{ring}_{2N+2}(\omega, D, 1) - \lambda I_{2N+2} \right). \]

For \( j = 1, \ldots, N \) the following relation between corresponding eigenvectors for the chain and the ring models holds:

\[ \vec{u}_j = \Pi^{2N+2}_N \vec{w}_j, \]

where for \( M > L \)

\[ \Pi^M_L : \mathbb{R}^M \rightarrow \mathbb{R}^L \]

is the projection onto the first \( L \)-coordinates.
4. Alternating models

In this section we compare alternating spin-1/2 chain and ring models, i.e. models of period 2. We will discuss only open spin chains with odd number of sites as the structure of this model in the even case contains transcendental equation [12] which does not feature in the ring model (see below).

To diagonalize the Hamiltonian of an open alternating linear spin-1/2 chain with odd number of sites we shall rewrite the initial three-diagonal matrix for the Hamiltonian

\[ H_{\text{chain}}^{2n-1}(\omega_1, \omega_2, D_1, D_2, 2) \]

in a different basis and represent it as a block 2 × 2 matrix with respect to odd \( u^{(1)} \) and even \( u^{(2)} \) components of vectors:

\[
H_{\text{chain}}^{2n-1}(\omega_1, \omega_2, D_1, D_2, 2) \begin{pmatrix} u^{(1)} \\ u^{(2)} \end{pmatrix} = \begin{bmatrix} 2\omega_1 I_n & L'_{\text{chain}} \\ L_{\text{chain}} & 2\omega_2 I_{n-1} \end{bmatrix} \begin{pmatrix} u^{(1)} \\ u^{(2)} \end{pmatrix}
\]

where

\[
L_{\text{chain}} : \mathbb{R}^n \rightarrow \mathbb{R}^{n-1};
\]

\[
L_{\text{chain}} = \begin{bmatrix}
D_1 & D_2 & 0 & \cdots & 0 & 0 & 0 \\
0 & D_1 & D_2 & \cdots & 0 & 0 & 0 \\
0 & 0 & D_1 & \ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & 0 & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & 0 & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & 0 & \ddots & \ddots & \ddots & \ddots
\end{bmatrix}.
\]

Observe that 2\( \omega_1 \) is an eigenvalue of \( H_{\text{chain}}^{2n-1}(\omega_1, \omega_2, D_1, D_2, 2) \) of multiplicity one with an eigenvector \( u \) having the following components:

\[
u^{(1)} \in \text{Ker} L_{\text{chain}}, \quad u^{(2)} = 0.
\]

If \( \lambda \neq 2\omega_1 \) is an eigenvalue for \( H_{\text{chain}}^{2n-1}(\omega_1, \omega_2, D_1, D_2, 2) \) then

\[
\begin{aligned}
u^{(1)} &= \frac{1}{\lambda - 2\omega_1} L'_{\text{chain}} u^{(2)}, \\
(\lambda - 2\omega_2) u^{(2)} &= L_{\text{chain}} L'_{\text{chain}} u^{(2)}.
\end{aligned}
\]

This implies that

\[
(\lambda - 2\omega_1)(\lambda - 2\omega_2) u^{(2)} = L_{\text{chain}} L'_{\text{chain}} u^{(2)}.
\]

\( L_{\text{chain}} L'_{\text{chain}} \) is a tridiagonal matrix with all elements on the main diagonal equal to \( D_1^2 + D_2^2 \) and all off-diagonal elements equal to \( D_1 D_2 \). Using explicit diagonalization of the Hamiltonian of a homogeneous chain from the previous section we deduce

**Theorem 3.** Each eigenvalue of the Hamiltonian \( H_{\text{chain}}^{2n-1}(\omega_1, \omega_2, D_1, D_2, 2) \) of an alternating spin system with odd number of sites is either \( 2\omega_1 \) or it is a solution of the equation

\[
det (H_{1,2} - \lambda I_2) - D_2^2 = 2D_1 D_2 \cos \left( \frac{\pi j}{n} \right), \quad j = 1, 2, \ldots, n - 1.
\]

All eigenvalues have multiplicity one and if \( \lambda \) is a root of (25) for some \( j = 1, 2, \ldots, n - 1 \), then it is an eigenvalue for \( H_{\text{chain}}^{2n-1}(\omega_1, \omega_2, D_1, D_2, 2) \) and the component \( u^{(2)} \) of the corresponding eigenvector \( u_\lambda \) is

\[
u^{(2)} = \left( \sin \left( \frac{\pi j}{n} \right), \ldots, \sin \left( \frac{(n-1)\pi j}{n} \right) \right).
\]

The other component \( u^{(1)} \) is given by:

\[
u^{(1)} = \frac{1}{\lambda - 2\omega_1} L'_{\text{chain}} u^{(2)}.
\]
An eigenvector corresponding to $2\omega_1$ has $u_{(2)} = 0$ and $u_{(1)}$ spans the one-dimensional kernel of $L_{\text{chain}}$.

**Remark 2.** Theorem 3 was discovered in [9]. The case of even number of sites in open alternating spin-$1/2$ chain models was solved in [12]. Arguments given before the statement of this theorem yield another proof of the result from [9].

Now we consider the ring case. Set $q_l = \exp \left( \frac{2\pi l}{n} \right)$, $l = 0, 1, \ldots, n - 1$ and

\[
U_l = (1, 0, q_l, 0, q_l^2, \ldots, q_l^{n-1}, 0), \quad V_l = (0, 1, 0, q_l, 0, \ldots, 0, q_l^{n-1}),
\]

then

\[
H_{2n}^{\text{ring}}(\omega_1, \omega_2, D_1, D_2, 2) U_l = 2\omega_1 U_l + (D_1 + D_2 q_l) V_l,
\]

\[
H_{2n}^{\text{ring}}(\omega_1, \omega_2, D_1, D_2, 2) V_l = (D_2 q_l^{-1} + D_1) U_l + 2\omega_2 V_l.
\]

Therefore, $\mu U_l + \kappa V_l$ is an eigenvector for $H_{2n}^{\text{ring}}$ with eigenvalue $\lambda$ if $(\mu, \kappa)$ is an eigenvector for

\[
\begin{pmatrix}
2\omega_1 & D_2 q_l^{-1} + D_1 \\
D_1 + D_2 q_l & 2\omega_2
\end{pmatrix}
\]

with eigenvalue $\lambda$. Because,

\[
(D_2 q_l^{-1} + D_1)(D_1 + D_2 q_l) = D_1^2 + D_2^2 + 2D_1 D_2 \cos \left( \frac{2\pi l}{n} \right) > 0
\]

we conclude that $2\omega_1$ is not an eigenvalue for $H_{2n}^{\text{ring}}$ and

\[
\mu = \frac{D_2 q_l^{-1} + D_1}{\lambda - 2\omega_1} \kappa.
\]

This leads to the following theorem.

**Theorem 4.** Each eigenvalue of the Hamiltonian $H_{2n}^{\text{ring}}(\omega_1, \omega_2, D_1, D_2, 2)$ is a solution to the equation

\[
\det (H_{1,2} - \lambda I_2) - D_2^2 = 2D_1 D_2 \cos \left( \frac{2\pi j}{n} \right)
\]

for some $0 \leq j \leq n/2$. If $\lambda_j$ is a solution to (34) with $0 < j < n/2$ then it is an eigenvalue of $H_{2n}^{\text{ring}}$ of multiplicity two. Components $u_{(2)}$ of the corresponding eigenvector $u_{\lambda_j}$ can be chosen as

\[
\left( \cos \left( \frac{2\pi j}{n} \right), \cos \left( \frac{2 \cdot 2\pi j}{n} \right), \ldots, \cos \left( \frac{(n - 1) \cdot 2\pi j}{n} \right), 1 \right),
\]

or

\[
\left( \sin \left( \frac{2\pi j}{n} \right), \sin \left( \frac{2 \cdot 2\pi j}{n} \right), \ldots, \sin \left( \frac{(n - 1) \cdot 2\pi j}{n} \right), 0 \right).
\]

If $\lambda_j$ is a solution to (34) with $j = 0$ or $j = n/2$ then it is an eigenvalue of $H_{2n}^{\text{ring}}$ of multiplicity one. For $j = 0$ the component $u_{(2)}$ can be chosen as

\[
u_{(2)} = (1, 1, 1, \ldots, 1, 1),
\]

and for $j = n/2$

\[
u_{(2)} = (1, -1, 1, -1, \ldots, 1, -1)
\]
In all cases

\[ u(1) = \frac{1}{\lambda - 2\omega_1} L_{\text{ring}}^t u(2), \]

where \( n \times n \) matrix \( L_{\text{ring}} \) is given by:

\[
L_{\text{ring}} = \begin{bmatrix}
D_1 & D_2 & 0 & \cdots & 0 & 0 \\
0 & D_1 & D_2 & \cdots & 0 & 0 \\
0 & 0 & D_1 & \ddots & \vdots & \vdots \\
\vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ddots & \ddots & \ddots \\
D_2 & 0 & 0 & \cdots & 0 & D_1
\end{bmatrix}.
\]

Remark 3. Theorem 4 was proved in [4] and [16]. Arguments given before the statement of the theorem comprise an alternative proof of this result.

Corollary 2. The spectra of \( H_{2n-1}^{\text{chain}}(\omega_1, \omega_2, D_1, D_2, 2) \) and \( H_{4n}^{\text{ring}}(\omega_1, \omega_2, D_1, D_2, 2) \) are related to each other by means of

\[
\det \left( H_{2n-1}^{\text{chain}}(\omega_1, \omega_2, D_1, D_2, 2) - \lambda I_{2n-1} \right)^2 \left( \det(H_{1,2} - \lambda I_2) - D_2^2 - 2D_1D_2 \right) \times \\
\det \left( H_{4n}^{\text{ring}}(\omega_1, \omega_2, D_1, D_2, 2) - \lambda I_{4n} \right) (2\omega_1 - \lambda)^2
\]

If \( u_j \) and \( v_j \) are eigenvectors of \( H_{2n-1}^{\text{chain}}(\omega_1, \omega_2, D_1, D_2, 2) \) and \( H_{4n}^{\text{ring}}(\omega_1, \omega_2, D_1, D_2, 2) \) respectively, corresponding to the same eigenvalue \( \lambda_j \), \( j = 1, 2, \ldots, n-1 \), and \( v_j \) is of the form (36) then

\[ u_j = \Pi_{2n-1} v_j. \]

Proof. The first part of the theorem comes from comparison of the spectra for \( H_{2n-1}^{\text{chain}} \) and \( H_{4n}^{\text{ring}} \) given in Theorems 3, 4. The second part is a consequence of the structure of the component \( u(2) \) of the corresponding eigenvectors (in particular, that the \( n \)-th coordinate of \( u(2) \) in the ring case is zero) and the fact that \( L_{\text{chain}} \) forms the \((n-1) \times n\)-left upper corner of \( L_{\text{ring}} \). \( \square \)

5. Diagonalization of an XY Hamiltonian of spin-1/2 rings with periodic coupling constants and Larmor frequencies

We now proceed with the most general case of periodic models and give an alternative to [5] diagonalization procedure for a Hamiltonian of a spin-1/2 ring with periodic coefficients of any period. Observe some elementary properties of quantum integrals for such systems. Let \( T_N : \mathbb{R}^N \to \mathbb{R}^N \) be

\[
T_N = \begin{bmatrix}
0 & 1 & 0 & \cdots & 0 & 0 \\
0 & 0 & 1 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 & 1 \\
1 & 0 & 0 & \cdots & 0 & 0
\end{bmatrix}.
\]

Performing explicitly matrix multiplication we deduce that

\[
T_{km} H_{km}^{\text{ring}}(\omega_1, \ldots, \omega_{k-1}, \omega_k, D_1, \ldots, D_{k-1}, D_k) T_{km}^t = \\
H_{km}^{\text{ring}}(\omega_2, \ldots, \omega_k, \omega_1, D_2, \ldots, D_k, D_1).
\]
In particular,
\[(T_{km})^k H_{km}^{\text{ring}} = H_{km}^{\text{ring}} (T_{km})^k.\]
Consider two collections of roots of one
\[p_j = e^{\frac{2\pi i j}{m}}, \quad j = 0, 1, \ldots, k - 1, \quad r_l = e^{\frac{2\pi i l}{m}}, \quad l = 0, 1, \ldots, m - 1,\]
and for each pair \((j, l)\), \(j = 0, 1, \ldots, k - 1, \quad l = 0, 1, \ldots, m - 1\), let us introduce a vector
\[V_{jl} = (1, p_j r_l, p_j^2 r_l^2, \ldots, p_j^{km-1} r_l^{km-1})^t.\]
Obviously,
\[T_{km} (V_{jl}) = p_j r_l V_{jl},\]
and, therefore, from commutation relation (45) \(\tilde{H}_{km} (V_{jl})\) belongs to a subspace spanned by \(V_{0,l}, \ldots, V_{k-1,l}\).

**Lemma 1.** A subspace of \(\mathbb{R}^{km}\) spanned by \(V_{0,l}, \ldots, V_{k-1,l}\) coincides with a subspace spanned by
\[(T_t^t) \left( V_t \right), \quad \ldots, \quad (T_t^t)^{k-1} \left( V_t \right),\]
where
\[V_t = (1, 0, \ldots, 0, q_t, 0, \ldots, 0, q_t^2, 0, \ldots, 0, q_t^{k-1}, 0, \ldots, 0)^t, \quad q_t = e^{\frac{2\pi i t}{m}}\]

**Proof.** Let us introduce vectors
\[U_j = (1, p_j, p_j^2, \ldots, p_j^{k-1})^t, \quad j = 0, 1, \ldots, k - 1,\]
and the corresponding Vandermonde \(k \times k\)-matrix
\[W_k = (U_0, U_1, \ldots, U_{k-1}).\]
Performing explicitly matrix multiplication we deduce that
\[(V_{0,t}, \ldots, V_{k-1,t}) W_k^{-1} = \left( \tilde{V}_t, r_t (T_t^t) \left( \tilde{V}_t \right), \ldots, r_t^{k-1} (T_t^t)^{k-1} \left( \tilde{V}_t \right) \right),\]
which implies the statement. \(\square\)

For every \(l = 0, \ldots, m - 1\) we define
\[H_k(q_l) = \begin{bmatrix}
2\omega_1 & D_1 & 0 & \cdots & 0 & q_l^{-1} D_k \\
D_1 & 2\omega_2 & D_2 & \cdots & 0 & 0 \\
0 & D_2 & 2\omega_3 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 2\omega_{k-1} & D_{k-1} \\
q_l D_k & 0 & 0 & \cdots & D_{k-1} & 2\omega_k
\end{bmatrix}.\]

**Theorem 5.** Each eigenvalue of \(H_{km}^{\text{ring}}(\omega_j, D_j, k)\) is an eigenvalue of \(H_k(q_l)\), for some \(l = 1, \ldots, m\). If \((\mu_1, \mu_2, \ldots, \mu_k)^t\) is an an eigenvector of \(H_k(q_l)\) then
\[\mu_1 \tilde{V}_t + \mu_2 (T_t^t) \left( \tilde{V}_t \right) + \cdots + \mu_k (T_t^t)^{k-1} \left( \tilde{V}_t \right),\]
with
\[\tilde{V}_t = (1, 0, \ldots, 0, q_t, 0, \ldots, 0, q_t^2, 0, \ldots, 0, q_t^{k-1}, 0, \ldots, 0)^t,\]
is an eigenvector of \(H_{km}^{\text{ring}}(\omega_j, D_j, k)\).
Proof. Note that $\mathcal{V}_l = (V_{0l}, V_{1l}, \ldots, V_{k-1,l})$ is invariant under $H_{km}^{ring}$ and, thus, we can work with each subspace $\mathcal{V}_l$ independently. Let $V \in \mathcal{V}_l$ be an eigenvector for $H_{km}^{ring}$ with eigenvalue $\kappa$. From Lemma 1 we can assume that

$$V = \mu_1 \tilde{V}_l + \mu_2 T_{km}^t (\tilde{V}_l) + \cdots + \mu_k (T_{km}^k)^{k-1} (\tilde{V}_l).$$

We shall verify that $(\mu_1, \mu_2, \ldots, \mu_k)$ is an eigenvector for $H_k(q_l)$ with the same eigenvalue $\kappa$. Indeed, look at the $(ks + t)$ row of $H_{km}^{ring}$, $0 \leq s \leq m - 1, 1 \leq t \leq k$. If $1 < t < k$ then multiplying it with $V$ we get

$$\mu_{t-1} q_l^s D_{t-1} + \mu_t q_l^s 2 \omega_t + \mu_{t+1} q_l^s D_t.$$

For $t = 1$ and $t = k$ we obtain respectively:

$$\mu_k q_l^{s-1} D_k + \mu_1 q_l^s 2 \omega_1 + \mu_2 q_l^s D_2,$$

and

$$\mu_{k-1} q_l^s D_{k-1} + \mu_k q_l^s 2 \omega_k + \mu_1 q_l^{s+1} D_k.$$

Comparing it with the $ks + t$ coordinate of $\kappa V$ and dividing both sides by $q_l^s$ we get exactly the $t$-th row of

$$(k)(H_k(q_l)(\mu_1, \ldots, \mu_k)^t = \kappa(\mu_1, \ldots, \mu_k)^t,$$

which is what we need. \hfill $\square$

Remark 4. Theorem 5 was proved in [5]. The proof of the result given above presents different approach compared to [5] where the authors used Fourier transform.

We finish this section with one useful lemma.

Lemma 2. The characteristic polynomial of $H_k(q_l)$ can be rewritten as:

$$\det(H_k(q_l) - \lambda I_k) = \det(H_{1,k} - \lambda I_k) - \det(H_{2,k-1} - \lambda I_{k-2}) D_k^2 - (-1)^k 2D_1 \cdots D_k \cos \left(\frac{2\pi l}{m}\right).$$

Proof. Consider $\det(H_k(q_l) - \lambda I_k)$ as a polynomial in $D_k$. It is a quadratic polynomial with free term

$$\det(H_{1,k} - \lambda I_k).$$

The coefficient of $D_k^2$ is

$$(-1)^{k+1+k-1+1} \det(H_{2,k-1} - \lambda I_{k-2})$$

and, finally, the coefficient of $D_k$ is

$$(-1)^{k+1} D_1 \cdots D_{k-1} (q_l + q_l^{-1}) = -(-1)^k 2D_1 \cdots D_{k-1} \cos \left(\frac{2\pi l}{m}\right).$$

$\square$
6. Comparison

In this section we give a comparison of periodic chain and ring models similar to Corollaries 1, 2 for any period \( k \). Let \( Q_{\text{chain}}, R_{\text{chain}} : \mathbb{R}^n \to \mathbb{R}^{n-1} \) be given by

\[
Q_{\text{chain}} = \begin{bmatrix}
1 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 1 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 1 & \ddots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 1 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 1 \\
\end{bmatrix}, \quad R_{\text{chain}} = \begin{bmatrix}
0 & 1 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 1 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \ddots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 1 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 1 \\
\end{bmatrix}.
\]

**Theorem 6.** Each eigenvalue of the Hamiltonian \( H_{\text{chain}}^{\text{ring}}(\omega_j, D_j, k) \) of a \( k \)-periodic system with \( kn - 1 \) sites is either an eigenvalue of \( H_{1,k-1} \) or it is a solution of the equation

\[
det(H_{1,k} - \lambda I_k) - \det(H_{2,k-1} - \lambda I_{k-2}) D_k^2 = (-1)^k 2D_1 \cdots D_k \cos \left( \frac{\pi j}{n} \right),
\]

for some \( j = 1, \ldots, n-1 \). Equation (67) does not have repeated roots and all \( k(n-1) \) solutions constructed from (67) are pairwise distinct and are not eigenvalues of \( H_{1,k-1} \).

If \( \lambda \) is the solution of (67) for some \( j = 1, \ldots, n-1 \), then it is an eigenvalue of \( H_{\text{chain}}^{\text{ring}}(\omega_j, D_j, k) \) and the component \( u(\lambda) \) of the corresponding eigenvector \( u_\lambda \) is

\[
u(\lambda) = \left( \sin \left( \frac{\pi j}{n} \right), \ldots, \sin \left( \frac{(n-1)\pi j}{n} \right) \right).
\]

The other components \( u(j), j = 1, \ldots, k-1 \), are determined uniquely from

\[
u(j) = \frac{(-1)^j}{\det(H_{1,k-1} - \lambda I_{k-1})} \cdot [D_1 \cdots D_{j-1} \det(H_{j+1,k-1} - \lambda I_{j-1}) \cdot D_k R'_{\text{chain}} + \frac{(-1)^k \det(H_{1,j-1} - \lambda I_{j-1}) D_{j+1} \cdots D_{k-1} Q'_{\text{chain}}}{\det(H_{1,k-1} - \lambda I_{k-1})} u(k),
\]

where \( Q_{\text{chain}}, R_{\text{chain}} \) are given in (66). Every eigenvalue \( \lambda \) of \( H_{1,k-1} \) is an eigenvalue of \( H \). The component \( u(k) \) of the corresponding eigenvector of \( H_{\text{chain}}^{\text{ring}}(\omega_j, D_j, k) \) is zero. The component \( u(1) \) spans the one-dimensional kernel of

\[
(-1)^{k-1} D_1 \cdots D_{k-2} D_{k-1} Q_{\text{chain}} - \det(H_{2,k-1} - \lambda I_{k-2}) R_{\text{chain}}.
\]

The remaining components \( u(j), j = 2, \ldots, k-1 \), are

\[
u(j) = \frac{(-1)^j}{\det(H_{2,k-1} - \lambda I_{k-2})} \cdot D_1 \cdots D_{j-1} \det(H_{j+1,k-1} - \lambda I_{j-1}) \cdot D_k R_{\text{chain}}
\]

**Remark 5.** A complete proof of this statement is given in [10].

**Theorem 7.** Each eigenvalue of \( H_{\text{ring}}^{\text{ring}}(\omega_j, D_j, k) \) is a solution of the equation

\[
det(H_{1,k} - \lambda I_k) - \det(H_{2,k-1} - \lambda I_{k-2}) D_k^2 = (-1)^k 2D_1 \cdots D_k \cos \left( \frac{2\pi l}{m} \right)
\]

for some \( 0 \leq l \leq m/2 \). If \( \lambda_l \) is a solution of (72) for some \( 0 < l < m/2 \), then it is an eigenvalue of \( H_{\text{ring}}^{\text{ring}}(\omega_j, D_j, k) \) of multiplicity 2 and the component \( u(k) \) of the corresponding eigenvector \( u_l \) is either

\[
\left( \cos \left( \frac{2\pi l}{m} \right), \cos \left( \frac{2 \cdot 2\pi l}{m} \right), \ldots, \cos \left( \frac{(m-1)2\pi l}{m} \right), 1 \right).
\]
or

\[
\left( \sin \left( \frac{2\pi l}{m} \right), \sin \left( \frac{2 \cdot 2\pi l}{m} \right), \ldots, \sin \left( \frac{(m-1)2\pi l}{m} \right), 0 \right).
\]

If \( \lambda_l \) is a solution to (34) with \( l = 0 \) or \( l = m/2 \) then it is an eigenvalue of \( H_{km}^{ring} \) of multiplicity one. For \( l = 0 \) the component \( u_{(k)} \) can be chosen as

\[
u_{(k)} = (1, 1, 1, \ldots, 1),
\]

and for \( l = m/2 \)

\[
u_{(k)} = (1, -1, 1, -1, \ldots, 1).
\]

In all cases the other components \( \nu_{(j)}, j = 1, \ldots, k - 1 \), are determined uniquely from

\[
u_{(j)} = \frac{(-1)^j}{\det (H_{1,k-1} - \lambda I_{k-1})} \left[ D_1 \cdots D_{j-1} \det (H_{j+1,k-1} - \lambda I_{j-1}) D_k T_m^t + \right.
\]

\[
+ \left( -1 \right)^k \det (H_{1,j-1} - \lambda I_{j-1}) D_j \cdots D_{k-2} D_{k-1} \nu_{(k)},
\]

where \( T_m \) is given by (43) \((N = m)\).

**Proof.** The eigenvalue part of the theorem is a consequence of Theorem 5 and Lemma 2. To understand the structure of eigenvectors we consider the matrix

\[
H_{i,j} = \left( \begin{array}{cc}
H_{1,k-1} & -\lambda I_{k-1} \\
-\lambda I_{k-1} & H_{1,k-1}
\end{array} \right),
\]

where \( \lambda \) is an eigenvalue. The following explicit expressions were deduced in [10] for \( t > s \)

\[
P_{i,s} = P_{s,t} = (-1)^{t+s} \frac{\det (H_{1,s-1} - \lambda I_{s-1}) D_s \cdots D_{t-1} \det (H_{t+1,k-1} - \lambda I_{t-1})}{\det (H_{1,k-1} - \lambda I_{k-1})},
\]

and

\[
P_{t,t} = \frac{\det (H_{1,t-1} - \lambda I_{t-1}) \det (H_{t+1,k-1} - \lambda I_{t-1})}{\det (H_{1,k-1} - \lambda I_{k-1})}.
\]

If \( \vec{v} = (\mu_1, \ldots, \mu_k) \) is an eigenvector for \( H_k(\vec{q}) \) with eigenvalue \( \lambda \) then for the matrix

\[
G = \left( \begin{array}{cc}
P & 0 \\
0 & 1
\end{array} \right)
\]

we have

\[
G \cdot (H_k(\vec{q}) - \lambda I_k) \vec{v} = 0,
\]

or in another form

\[
\begin{pmatrix}
1 & 0 & \cdots & 0 & 0 \\
0 & 1 & \cdots & 0 & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & 0 & \cdots & 1 & 0 \\
D_k q_l & 0 & \cdots & 0 & D_{k-1}
\end{pmatrix}
\begin{pmatrix}
D_k q_l^{-1} \\
0 \\
\vdots \\
0 \\
D_{k-1}
\end{pmatrix}
\begin{pmatrix}
\mu_1 \\
\mu_2 \\
\vdots \\
\mu_{k-2} \\
\mu_{k-1} \\
\mu_k
\end{pmatrix}
= 0.
\]

This implies that

\[
\mu_j = - (P_{j,1} D_k q_l^{-1} + P_{j,k-1} D_{k-1}) \mu_k.
\]

Substituting this into (55) and taking into account (78), (79) we obtain (77). \( \square \)
Corollary 3. The spectra of $H_{km-1}^{\text{chain}}(\omega_j, D_j, k)$ and $H_{2km}^{\text{ring}}(\omega_j, D_j, k)$ are related to each other by means of

$$
\det \left( H_{km-1}^{\text{chain}}(\omega_j, D_j, k) - \lambda I_{km-1} \right) \times \\
\times (\det(H_{1,k} - \lambda I_k) - \det(H_{3,k-1} - \lambda I_{k-2})D_k^2 - 2D_1 \cdots D_k) \times \\
\times (\det(H_{1,k} - \lambda I_k) - \det(H_{2,k-1} - \lambda I_{k-2})D_k^2 + 2D_1 \cdots D_k) = \\
= \det \left( H_{2km}^{\text{ring}}(\omega_j, D_j, k) - \lambda I_{2km} \right) \det(H_{1,k-1} - \lambda I_{k-1})^2
$$

If $u_j$ and $v_j$ are eigenvectors of $H_{km-1}^{\text{chain}}(\omega_j, D_j, k)$ and $H_{2km}^{\text{ring}}(\omega_j, D_j, k)$ respectively, corresponding to the same eigenvalue $\lambda_j$, $j = 1, 2, \ldots, m - 1$, and $v_j$ is of the form (74) then

$$u_j = \Pi_{2km-1}^{\text{chain}} v_j.$$

Proof. The proof repeats the proof of Corollary 2. The eigenvalue part is a direct consequence of the structure of the spectra from Theorems 6, 7. The eigenvector part is a consequence of the formulae (69) and (77), because matrix $Q_{\text{chain}}$ is a left upper corner of $I_{2m}$, $K_{\text{chain}}$ is a left upper corner of $T_m$, $u(k)$ from Theorem 6 forms the first $m - 1$ coordinates of $u(k)$ from (74), and the $m$-th coordinate of $u(k)$ from (74) is zero.

7. Conclusion

We gave an explicit comparison of the spectrum properties of the XY Hamiltonians of open spin chain and closed spin ring models with periodic in space coefficients and identified the part of spectra responsible for the reflection of spin wave packets from the ends of the chain and for the translation symmetry of the ring. Common parts of the spectra for $k$-periodic chain with $kn - 1$ sites and $k$-periodic ring with $2kn$ sites correspond to the same evolution of these systems at short times.

One can argue that a similar type of behavior must be featured in other one-dimensional spin systems including the one-dimensional Ising model in the transverse magnetic field. In particular, using a recent solution of a periodic Ising model on a ring in [6] we might be able to recover an exact diagonalization for the Hamiltonian of the corresponding model on an open chain. Experimental results [13] yield another perspective of the development of these analytical findings. Some problems of quantum information theory (for example, boundary effects in the study of entanglement in one-dimensional systems [15], or relations between entanglement and qubit addressing [8]) provide new possible applications of the methods suggested.

References


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