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Exact diagonalization of the XY-Hamiltonian of open linear chains with periodic coupling constants and its application

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Abstract

A new method of diagonalization of the XY-Hamiltonian of inhomogeneous open linear chains with periodic (in space) changing Larmor frequencies and coupling constants is developed. As an example of application, multiple-quantum dynamics of an inhomogeneous chain consisting of 1001 spins is investigated. Intensities of multiple-quantum coherences are calculated for arbitrary inhomogeneous chains in the approximation of the next-nearest interactions.

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1. Introduction

One-dimensional exactly solvable models (spin chains, rings) [1] have been actively employed for studying various problems of spin dynamics [2] and quantum information theory [3]. Substantial progress in our understanding of spin dynamics has been achieved on the basis of a homogeneous XY model for spin chains ($s = 1/2$) in the transverse magnetic field [4, 5]. Recently, Hamiltonians of the simplest inhomogeneous systems (alternating systems) have been diagonalized for the ring [6] and the linear spin chain [7]. Development of methods for exact solution of inhomogeneous spin problems has become especially urgent in conjunction with recent progress in quantum computation and quantum information theories [3]. In particular, these methods can be used for studying the quantum state transfer from one end of the chain to another one [8, 9]. The qubit addressing problem can be attacked by variation of the Larmor frequencies of different spins [10] in classical one-dimensional models. This immediately brings inhomogeneity into the XY model as diagonal elements of the corresponding Hamiltonian are not equal. Consequently, we arrive at one-dimensional spin models with Hamiltonians described by three-diagonal matrices which elements on the diagonal are not equal, and those under and over the main diagonal are not identically equal

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as well. Low sensitivity of nuclear magnetic resonance (NMR), which is widely applied in experimental implementation of quantum computations [3], leads to a further complication of the model described above. Consideration of k-qubit systems brings us naturally to the study of $kn+r$ spin chains ($r < k$, n is arbitrary and k, n, r are non-negative integers), with Larmor frequencies and constants of spin–spin interactions repeating periodically with period k.

The paper suggests a new method of diagonalization of a Hamiltonian of a linear k-periodic spin chain of length $kn+r$ for various values $r < k$. Special attention is given to the case $k = 3$. For a spin chain of $(3n+2)$-sites with periodic parameters (period 3), a multiple-quantum dynamics [2, 11] is analysed and intensities of all MQ coherences are calculated (see figure 2). This analysis is based on the explicit diagonalization of the Hamiltonian of a linear three-periodic spin chain with $(3n+2)$-sites (theorem 5.1) and the exact formulae, obtained in the paper (theorem 6.1), for the intensities of all MQ coherences developed in any nuclear spin system coupled by the nearest-neighbour dipolar interactions. We conclude the paper with a discussion of the properties of eigenvalues and eigenvectors of the general k-periodic systems with $(kn-1)$-sites (theorem 7.1).

2. Model

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

$$H = \sum_{n=1}^{N} \omega_n I_{nz} + \sum_{n=1}^{N-1} D_{n,n+1}(I_{n,x}I_{n+1,x} + I_{n,y}I_{n+1,y}), \qquad (1)$$

where ω_n, $n = 1, \ldots, N$, are the Larmor frequencies, and $D_{n,n+1}$, $n = 1, \ldots, N-1$, are the NN coupling constants. The Jordan–Wigner transformation [4] allows one to study all the properties of such a system by means of a diagonalization of the matrix $D + 2\Omega$ with

$$\Omega = \begin{bmatrix} \omega_1 & 0 & \cdots & 0 & 0 \\ 0 & \omega_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \omega_{N-1} & 0 \\ 0 & 0 & \cdots & 0 & \omega_N \end{bmatrix}, \qquad D = \begin{bmatrix} 0 & D_1 & \cdots & 0 & 0 \\ D_1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & D_{N-1} \\ 0 & 0 & \cdots & D_{N-1} & 0 \end{bmatrix}. \qquad (2)$$

The problem of diagonalization of $D+2\Omega$ with arbitrary constants ω_n, $n = 1, \ldots, N$, and D_k, $k = 1, \ldots, N-1$, for large N ($N \sim 10^6$) and computation of various functions of $D+2\Omega$ is a time-consuming problem usually dealt with the help of super computers. On the other hand, there are two known exact solutions (suitable for studying systems with large N) for such a problem when the spin system considered has periodic changing Larmor frequencies and coupling constants. Namely, the case of equal sites ($\omega_1 = \cdots = \omega_n = a$, $D_1 = \cdots = D_{N-1} = c$) has been solved in [4], while the case of period 2 with odd N ($\omega_1 = \omega_3 = \cdots = \omega_N$, $\omega_2 = \omega_4 = \cdots = \omega_{N-1}$, $D_1 = D_3 = \cdots = D_{N-2}$, $D_2 = D_4 = \cdots = D_{N-1}$) has been solved in [7].

The present paper concerns properties of a general periodic chain. In the following sections, we shall demonstrate how to reduce the diagonalization problem of the Hamiltonian of a k-periodic chain with $(kn-1)$-sites ($k > 2, n > 1$) to the problem of finding roots for explicitly given polynomials of degree less than or equal to k. Therefore, the methods developed are particularly useful when $n \gg k$.

In what follows we will utilize essentially the result on diagonalization of the homogeneous (in other words, 1-periodic) chain [4] which we state now.

Lemma 2.1. *Let $c \neq 0$, then the matrix*

$$J_n(a,c) = \begin{bmatrix} a & c & 0 & \cdots & 0 & 0 & 0 \\ c & a & c & \cdots & 0 & 0 & 0 \\ 0 & c & a & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & a & c & 0 \\ 0 & 0 & 0 & \cdots & c & a & c \\ 0 & 0 & 0 & \cdots & 0 & c & a \end{bmatrix} \tag{3}$$

has n-distinct eigenvalues

$$\lambda_j = a + 2c\cos\left(\frac{\pi j}{n+1}\right), \qquad j = 1, \ldots, n, \tag{4}$$

and the corresponding eigenvectors are of the form

$$\vec{x}_j = \left(\sin\left(\frac{\pi j}{n+1}\right), \sin\left(\frac{2\pi j}{n+1}\right), \ldots, \sin\left(\frac{n\pi j}{n+1}\right)\right). \tag{5}$$

Proof. It is a straightforward verification. □

3. Reduction over the period

Let us consider an open periodic chain of $(kn+d)$-sites $(k > d \geqslant 0, k > 1)$ with k-periodic nonzero NN coupling constants

$$\begin{aligned} &D_1 = D_{k+1} = \cdots = D_{kn+1}, && D_d = D_{k+d} = \cdots = D_{kn+d}, \\ &D_{d+1} = D_{k+d+1} = \cdots = D_{k(n-1)+d+1}, && D_k = D_{2k} = \cdots = D_{kn}, \end{aligned} \tag{6}$$

and k-periodic Larmor frequencies

$$\begin{aligned} &\omega_1 = \omega_{k+1} = \cdots = \omega_{kn+1}, && \omega_d = \omega_{k+d} = \cdots = \omega_{kn+d}, \\ &\omega_{d+1} = \omega_{k+d+1} = \cdots = \omega_{k(n-1)+d+1}, && \omega_k = \omega_{2k} = \cdots = \omega_{kn}, \end{aligned} \tag{7}$$

$(D_i, \omega_j \in \mathbb{R}, D_i \neq 0, i, j = 1, \ldots, k)$. We shall demonstrate how to reduce the diagonalization problem for the Hamiltonian of such a system to the problem of diagonalizing of a certain $k \times k$ block matrix which entries are matrices of dimensions $m \times m$, $(m+1) \times (m+1)$, $m \times (m+1)$ and $(m+1) \times m$ ($m = n$ in section 5 and $m = n-1$ in section 7). A particular case of this reduction will be used in the consecutive sections for studying k-periodic chains of length $kn - 1$.

Before we proceed we make an agreement regarding our notation. If a Gothic letter is used in the description of any matrix as its element, then this means that the corresponding place in the matrix is a matrix. The size and the structure of a matrix denoted by a Gothic letter should be clear or given in the context. Therefore, the original matrix is a block matrix. To underline that the matrix consists of blocks we shall often denote such matrices in bold. We shall also denote by I_m the $m \times m$ identity matrix.

The Hamiltonian of a k-periodic system with $(kn+d)$-sites has the following form:

$$H = D + 2\Omega, \tag{8}$$

where

$$\Omega = \begin{bmatrix} \omega_1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 \\ 0 & \omega_2 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \omega_{k-1} & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & \omega_k & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & \omega_1 & \cdots & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & \omega_k & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \omega_1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & \omega_{d-1} & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & \omega_d \end{bmatrix} \tag{9}$$

and

$$D = \begin{bmatrix} 0 & D_1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 \\ D_1 & 0 & D_2 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 \\ 0 & D_2 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & D_{k-1} & 0 & \cdots & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & D_{k-1} & 0 & D_k & \cdots & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & D_k & 0 & \cdots & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & D_{d-1} \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & D_{d-1} & 0 \end{bmatrix}. \tag{10}$$

To diagonalize the matrix H, one finds (real) eigenvectors u_ν and (real) eigenvalues λ_ν, $\nu = 1, \ldots, kn + d$, which satisfy the following equation:

$$(D + 2\Omega)u_\nu = \lambda_\nu u_\nu. \tag{11}$$

To resolve this equation we associate with each vector $u \in \mathbb{R}^{kn+d}$ vectors $u_{(j)}$, $j = 1, \ldots, k$, formed by those coordinates of u whose numbers have residue j modulo k. Observe that among vectors $u_{(1)}, \ldots, u_{(k)}$ there are d-vectors of dimension $(n + 1)$ and $(k - d)$-vectors of dimension n. Now equation (11) can be rewritten as a system of n linear equations in $u_{(j)}$:

$$\mathbf{H} \begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix} = \lambda_\nu \begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix} \tag{12}$$

with matrix $\mathbf{H} = 2\mathbf{\Omega} + \mathbf{D}$. Here

$$\mathbf{\Omega} = \begin{bmatrix} \mathcal{W}_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \mathcal{W}_2 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \mathcal{W}_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \mathcal{W}_{k-1} & 0 \\ 0 & 0 & 0 & \cdots & 0 & \mathcal{W}_k \end{bmatrix}, \tag{13}$$

$\mathcal{W}_j = \omega_j I_{n+1}$ for $j = 1, \ldots, d$, $\mathcal{W}_j = \omega_j I_n$ for $j = d+1, \ldots, k$, and with an exception of two degenerate cases

$$\mathbf{D} = \begin{bmatrix} 0 & \mathcal{D}_1 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & \mathcal{D}_k^t \\ \mathcal{D}_1 & 0 & \mathcal{D}_2 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \mathcal{D}_2 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \mathcal{D}_{d-1} & 0 & \mathcal{D}_d^t & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & \mathcal{D}_d & 0 & \mathcal{D}_{d+1} & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & \mathcal{D}_{d+1} & 0 & \mathcal{D}_{d+2} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \ddots & \ddots & \mathcal{D}_{k-2} & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \ddots & 0 & \mathcal{D}_{k-1} \\ \mathcal{D}_k & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & \mathcal{D}_{k-1} & 0 \end{bmatrix}, \tag{14}$$

with $\mathcal{D}_j = D_j I_{n+1}$ for $j = 1, 2, \ldots, d-1$, $\mathcal{D}_j = D_j I_n$ for $j = d+1, \ldots, k-1$, and $\mathcal{D}_d, \mathcal{D}_k : \mathbb{R}^{n+1} \to \mathbb{R}^n$ given by

$$\mathcal{D}_d = \begin{bmatrix} D_d & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & D_d & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & D_d & \ddots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & D_d & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & D_d & 0 \end{bmatrix},$$

$$\mathcal{D}_k = \begin{bmatrix} 0 & D_k & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & D_k & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & D_k & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & D_k \end{bmatrix}. \tag{15}$$

It is easy to see that

$$\mathcal{D}_d \mathcal{D}_d^t = D_d^2 I_n, \qquad \mathcal{D}_k \mathcal{D}_k^t = D_k^2 I_n, \qquad \mathcal{D}_d \mathcal{D}_k^t = D_d D_k J_n^t, \qquad \mathcal{D}_k \mathcal{D}_d^t = D_k D_d J_n, \tag{16}$$

where J_n is the Jordan $n \times n$ cell:

$$J_n = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ddots & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}. \tag{17}$$

There are two degenerate cases. In the case $k = 2$, matrix $\mathbf{D}$ decomposes as

$$\mathbf{D} = \begin{bmatrix} 0 & \mathcal{L}^t \\ \mathcal{L} & 0 \end{bmatrix}, \tag{18}$$

where $\mathcal{L} : \mathbb{R}^{n+d} \to \mathbb{R}^n$:

$$\mathcal{L} = \begin{bmatrix} D_1 & D_2 & 0 & \cdots & 0 & 0 & 0 \\ 0 & D_1 & D_2 & \cdots & 0 & 0 & 0 \\ 0 & 0 & D_1 & \ddots & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \ddots & \ddots \end{bmatrix}, \tag{19}$$

while in the case $k > 2$ and $d = 0$ we do not get matrix $\mathcal{D}_d$, and matrix $\mathcal{D}_k : \mathbb{R}^n \to \mathbb{R}^n$ is of the form

$$\mathcal{D}_k = \begin{bmatrix} 0 & D_k & 0 & \cdots & 0 & 0 \\ 0 & 0 & D_k & \cdots & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & D_k \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}. \tag{20}$$

It is easy to see that this matrix satisfies $\mathcal{D}_k \mathcal{D}_k^t = D_k^2 I_{n-1,1}$ for a diagonal matrix $I_{n-1,1}$ with the first $n-1$ diagonal elements equal to 1 and the last one equals 0.

Remark 3.1. From the reduction obtained above, we divide consideration of the diagonalization problem into three different cases: period $k = 2, 3$ and $k \geqslant 4$. In each case there are further reductions depending on the value of d. In the next sections, we shall work out the case $k \geqslant 3$ and $d = k - 1$.

4. Some auxiliary results

The diagonalization process of sections 5 and 7 will relay on some elementary facts about matrices of the form $H_{i,j} - \lambda I_{j-i+1}$, where for $i < j$:

$$H_{i,j} = \begin{bmatrix} 2\omega_i & D_i & 0 & \cdots & 0 & 0 \\ D_i & 2\omega_{i+1} & D_{i+1} & \cdots & 0 & 0 \\ 0 & D_{i+1} & 2\omega_{i+2} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2\omega_{j-1} & D_{j-1} \\ 0 & 0 & 0 & \cdots & D_{j-1} & 2\omega_j \end{bmatrix}. \tag{21}$$

These facts are mostly known and we give their proofs only for the reader's convenience.

Lemma 4.1. *If $D_s \neq 0$ for all $s = i, \ldots, j-1$, then all the eigenvalues of the matrix $H_{i,j}$ are distinct.*

Proof. Under the assumption that all D_s, $s = i, \ldots, j$, are nonzero, one can reconstruct every eigenvector u_ν of $H_{i,j}$ by its eigenvalue λ_ν and the first coordinate u_1. Moreover, the expressions for all other coordinates u_s, $s = 2, \ldots, j-i+1$, of u_ν are linear in u_1. This implies that every two eigenvectors u_ν and u'_ν with the same eigenvalue λ_ν are proportional with the coefficient u_1/u'_1. □

Lemma 4.2. *Non-diagonal elements of the adjoint matrix of* $(H_{i,j} - \lambda I_{j-i+1})$ *are*

$$\begin{aligned}\mathrm{adj}_{s,t}\{(H_{i,j} - \lambda I_{j-i+1})\} &= \mathrm{adj}_{t,s}\{(H_{i,j} - \lambda I_{j-i+1})\}\\ &= (-1)^{s+t}\det(H_{i,i+s-2} - \lambda I_{s-1})D_{i+s-1}\cdots D_{i+t-2}\det(H_{i+t,j} - \lambda I_{j-i-t+1}),\end{aligned} \quad (22)$$

where the first index in $\mathrm{adj}_{s,t}\{\cdot\}$ *denotes the row number, the second denotes the column number and* $t > s$. *The diagonal elements of the adjoint matrix are*

$$\mathrm{adj}_{s,s}\{(H_{i,j} - \lambda I_{j-i+1})\} = \det(H_{i,i+s-1} - \lambda I_{s-1})\det(H_{i+s+1,j} - \lambda I_{j-i-s}). \quad (23)$$

Proof. The first part follows from an observation that element D_{i+s-2} situated in row $(s-1)$ and column s of matrix $(H_{i,j} - \lambda I_{j-i+1})$ does not contribute to the cofactor (s, t) of $(H_{i,j} - \lambda I_{j-i+1})$, and similarly for element D_{i+t-1} situated in row t and column $(t+1)$. The second part is due to the splitting of the complement to the element (s, s) of $(H_{i,j} - \lambda I_{j-i+1})$ into $(H_{i,i+s-1} - \lambda I_{s-1})$ and $(H_{i+s+1,j} - \lambda I_{j-i-s})$. □

Corollary 4.1. *If we denote elements of* $(H_{i,j} - \lambda I_{j-i+1})^{-1}$ *by* $P_{s,t}$ *(where s is row, and t is column), then for* $t > s$

$$P_{t,s} = P_{s,t} = (-1)^{s+t}\frac{\det(H_{i,i+s-2} - \lambda I_{s-1})D_{i+s-1}\cdots D_{i+t-2}\det(H_{i+t,j} - \lambda I_{j-i-t+1})}{\det(H_{i,j} - \lambda I_{j-i+1})}. \quad (24)$$

The diagonal terms $P_{t,t}$ *are*

$$P_{t,t} = \frac{\det(H_{i,i+t-1} - \lambda I_{t-1})\det(H_{i+t+1,j} - \lambda I_{j-i-t})}{\det(H_{i,j} - \lambda I_{j-i+1})}. \quad (25)$$

Lemma 4.3. *If* $D_1 \neq 0$, *then matrices* $H_{1,k}$ *and* $H_{2,k}$ $(k \geqslant 2)$ *have no common eigenvalues.*

Proof. First, observe that it is true for $k = 2$:

$$\det(H_{1,2} - \lambda I_2) = (2\omega_1 - \lambda)(2\omega_2 - \lambda) - D_1^2, \quad (26)$$

and if λ is a root of $\det(H_{2,2} - \lambda I_1) = 0$, then $\lambda = 2\omega_2$, which is the root of

$$(2\omega_1 - \lambda)(2\omega_2 - \lambda) - D_1^2 = 0 \quad (27)$$

only if $D_1 = 0$.

For general k, if λ is a root of

$$\det(H_{2,k} - \lambda I_{k-1}) = 0, \quad (28)$$

then for such λ:

$$\begin{aligned}\det(H_{1,k} - \lambda I_k) &= (2\omega_1 - \lambda)\det(H_{2,k} - \lambda I_{k-1}) - D_1^2\det(H_{3,k} - \lambda I_{k-2})\\ &= -D_1^2\det(H_{3,k} - \lambda I_{k-2}).\end{aligned} \quad (29)$$

For the last polynomial, we can assume that it is nonzero by inductive hypothesis and because $D_1 \neq 0$. From here the statement follows. □

5. Exact diagonalization for a spin chain with $(3n + 2)$-sites

To demonstrate how the reduction over the period works, first we study a partial case of the main result, namely a chain of period 3 with $(3n + 2)$-sites. The reduction of section 3 leads us to the following system of linear equations:

$$\begin{bmatrix} 2\mathcal{W}_1 - \lambda_\nu I_{n+1} & \mathcal{D}_1 & \mathcal{D}_3^t \\ \mathcal{D}_1 & 2\mathcal{W}_2 - \lambda_\nu I_{n+1} & \mathcal{D}_2^t \\ \mathcal{D}_3 & \mathcal{D}_2 & 2\mathcal{W}_3 - \lambda_\nu I_n \end{bmatrix} \begin{bmatrix} u_{(1)} \\ u_{(2)} \\ u_{(3)} \end{bmatrix} = 0. \tag{30}$$

Recall that $\mathcal{W}_j$, $j = 1, 2, 3$, are just scalar matrices, as well as the matrix $\mathcal{D}_1$, while $\mathcal{D}_2, \mathcal{D}_3 : \mathbb{R}^{n+1} \to \mathbb{R}^n$ are given below:

$$\begin{aligned} \mathcal{D}_2 &= \begin{bmatrix} D_2 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & D_2 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & D_2 & \ddots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & D_2 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & D_2 & 0 \end{bmatrix}, \\ \mathcal{D}_3 &= \begin{bmatrix} 0 & D_3 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & D_3 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & D_3 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & D_3 \end{bmatrix}. \end{aligned} \tag{31}$$

From the second equation of (30)

$$(\lambda_\nu - 2\omega_2)u_{(2)} = \mathcal{D}_1 u_{(1)} + \mathcal{D}_2^t u_{(3)}. \tag{32}$$

Assume that an eigenvalue λ_ν of H is not equal to $2w_2$, then

$$u_{(2)} = \frac{D_1}{\lambda_\nu - 2\omega_2} u_{(1)} + \frac{1}{\lambda_\nu - 2\omega_2} \mathcal{D}_2^t u_{(3)}. \tag{33}$$

Substituting $u_{(2)}$ into the first equation and into the third equation of (30), and using that $\mathcal{D}_2 \mathcal{D}_2^t = D_2^2 I_n$ we obtain a system:

$$\begin{cases} \left(D_1^2 - (\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2)\right) u_{(1)} + \left(D_1 \mathcal{D}_2^t + (\lambda_\nu - 2\omega_2)\mathcal{D}_3^t\right) u_{(3)} = 0, \\ ((\lambda_\nu - 2\omega_2)\mathcal{D}_3 + D_1 \mathcal{D}_2) u_{(1)} + \left(D_2^2 - (\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_3)\right) u_{(3)} = 0. \end{cases} \tag{34}$$

Lemma 5.1. *If*

$$(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) \neq D_1^2, \tag{35}$$

then the following inequality holds

$$(\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_3) \neq D_2^2. \tag{36}$$

Proof. Observe, that if $\lambda_\nu = 2\omega_2$, then

$$(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) = 0 \neq D_1^2 \tag{37}$$

and

$$(\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_1) = 0 \neq D_2^2. \tag{38}$$

Therefore, it is left to consider the case when $\lambda_\nu \neq 2\omega_2$. Assume that

$$(\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_3) = D_2^2. \tag{39}$$

Then from the second equation of (34)

$$((\lambda_\nu - 2\omega_2)\mathcal{D}_3 + D_1\mathcal{D}_2)u_{(1)} = 0. \tag{40}$$

With respect to the standard scalar product $\langle\cdot,\cdot\rangle_{\mathbb{R}^m}$, $m = n, n+1$, we have

$$0 = \langle u_{(3)}, ((\lambda_\nu - 2w_2)\mathcal{D}_3 + D_1\mathcal{D}_2)u_{(1)}\rangle_{\mathbb{R}^n} = \left\langle \left(D_1\mathcal{D}_2^t + (\lambda_\nu - 2\omega_2)\mathcal{D}_3^t\right)u_{(3)}, u_{(1)}\right\rangle_{\mathbb{R}^{n+1}}. \tag{41}$$

Therefore, in order to satisfy the first equation of (34) we necessarily have

$$\begin{cases} \left(D_1^2 - (\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2)\right) u_{(1)} = 0, \\ \left(D_1\mathcal{D}_2^t + (\lambda_\nu - 2\omega_2)\mathcal{D}_3^t\right) u_{(3)} = 0. \end{cases} \tag{42}$$

From here and under the assumption that

$$(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) \neq D_1^2, \tag{43}$$

we obtain that $u_{(1)} = 0$. Because $D_j \neq 0$, $j = 1, 2, 3$, the matrix

$$\left(D_1\mathcal{D}_2^t + (\lambda_\nu - 2\omega_2)\mathcal{D}_3^t\right) \tag{44}$$

has rank n and its kernel is 0. Therefore, $u_{(3)} = 0$. Finally, from (33) we obtain that $u_{(2)} = 0$ and, thus, λ_ν is not an eigenvalue for H. This verifies the lemma. □

Assume as in lemma 5.1 that

$$(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) \neq D_1^2, \tag{45}$$

then from the first equation of (34) we deduce that

$$u_{(1)} = \frac{D_1\mathcal{D}_2^t + (\lambda_\nu - 2\omega_2)\mathcal{D}_3^t}{(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) - D_1^2} u_{(3)}. \tag{46}$$

Substituting (46) into (33) we obtain

$$u_{(2)} = \frac{(\lambda_\nu - 2\omega_1)\mathcal{D}_2^t + D_1\mathcal{D}_3^t}{(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) - D_1^2} u_{(3)}. \tag{47}$$

Due to lemma 5.1

$$(\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_3) \neq D_2^2. \tag{48}$$

Thus, from the second equation of (34) we have that

$$u_{(3)} = \frac{(\lambda_\nu - 2\omega_2)\mathcal{D}_3 + D_1\mathcal{D}_2}{(\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_3) - D_2^2} u_{(1)}. \tag{49}$$

Therefore, because $\lambda_\nu \neq 2\omega_2$, $u_{(3)}$ satisfies

$$\begin{aligned} &\left((\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_3) - (\lambda_\nu - 2\omega_3)D_1^2 - (\lambda_\nu - 2\omega_1)D_2^2 - (\lambda_\nu - 2\omega_2)D_3^2\right) u_{(3)} \\ &\quad = \left(D_1\mathcal{D}_3\mathcal{D}_2^t + D_1\mathcal{D}_2\mathcal{D}_3^t\right) u_{(3)}. \end{aligned} \tag{50}$$

This leads us to the following theorem:

Theorem 5.1. *For $j = 1, \ldots, n$ each of the three solutions of the cubic equation*

$$\begin{aligned} &(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_3) - (\lambda_\nu - 2\omega_2)D_3^2 - (\lambda_\nu - 2\omega_1)D_2^2 - (\lambda_\nu - 2\omega_3)D_1^2 \\ &\quad = 2D_1D_2D_3\cos\left(\frac{\pi j}{n+1}\right) \end{aligned} \tag{51}$$

is an eigenvalue for H. The component $u_{(3)}$ of the corresponding eigenvector u_ν is

$$u_{(3)} = \left(\sin\left(\frac{\pi j}{n+1}\right), \sin\left(\frac{2\pi j}{n+1}\right), \dots, \sin\left(\frac{n\pi j}{n+1}\right)\right). \tag{52}$$

The remaining components $u_{(1)}$ and $u_{(2)}$ are determined uniquely from

$$u_{(1)} = \frac{(\lambda_\nu - 2\omega_2)\mathcal{D}_3^t + D_1\mathcal{D}_2^t}{(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) - D_1^2} u_{(3)}, \tag{53}$$

and

$$u_{(2)} = \frac{(\lambda_\nu - 2\omega_1)\mathcal{D}_2^t + D_1\mathcal{D}_3^t}{(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) - D_1^2} u_{(3)}, \tag{54}$$

where $\mathcal{D}_2$, $\mathcal{D}_3$ are given in (31).

There are two other eigenvalues of H which satisfy the following quadratic equation:

$$(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) - D_1^2 = 0. \tag{55}$$

The component $u_{(3)}$ of the corresponding eigenvector u_ν is necessarily zero; the component $u_{(1)}$ spans the (one dimensional) kernel of

$$(\lambda_\nu - 2\omega_2)\mathcal{D}_3 + D_1\mathcal{D}_2 \tag{56}$$

and the component $u_{(2)}$ is

$$u_{(2)} = \frac{D_1}{\lambda_\nu - 2\omega_2} u_{(1)}. \tag{57}$$

All eigenvalues constructed are distinct and they exhaust all $(3n+2)$-distinct eigenvalues for H.

Proof. Let us consider the case when $2w_2$ is an eigenvalue for H and u_ν is the corresponding eigenvector. Then for the components $u_{(1)}$ and $u_{(3)}$ we have from the second equation of (30):

$$u_{(1)} = -\frac{1}{D_1}\mathcal{D}_2^t u_{(3)}. \tag{58}$$

From the first equation of (30)

$$u_{(2)} = -\frac{1}{D_1}\left(\frac{2\omega_2 - 2\omega_1}{D_1}\mathcal{D}_2^t + \mathcal{D}_3^t\right) u_{(3)}. \tag{59}$$

Substituting this into the third equation of (30), we obtain

$$\begin{aligned}\left(-\frac{1}{D_1}\mathcal{D}_3\mathcal{D}_2^t + -\frac{1}{D_1}\left(\frac{2\omega_2 - 2\omega_1}{D_1}\mathcal{D}_2\mathcal{D}_2^t + \mathcal{D}_2\mathcal{D}_3^t\right) + (2\omega_3 - 2\omega_2)\right) u_{(3)} \\ = \left((2\omega_3 - 2\omega_2) - (2\omega_2 - 2\omega_1)\frac{D_2^2}{D_1^2} - \frac{D_2 D_3}{D_1}\left(J_n + J_n^t\right)\right) u_{(3)} = 0.\end{aligned} \tag{60}$$

Thus, from lemma 2.1

$$2(\omega_3 - \omega_2)D_1^2 + 2(\omega_1 - \omega_2)D_2^2 - 2D_1D_2D_3\cos\left(\frac{\pi j}{n+1}\right) = 0, \tag{61}$$

for some $j = 1, \dots, n$. From here it follows that $2\omega_2$ also satisfies equation (51); moreover, the formulae for the component $u_{(3)}$ and (as a consequence) for $u_{(1)}$ and $u_{(2)}$ coincide with those given in the body of the theorem. We obtain that the case $\lambda_\nu = 2\omega_2$ can be considered simultaneously with all the other solutions of (51).

Therefore, every eigenvalue for H is either a solution for

$$(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) = D_1^2, \tag{62}$$

or it is a solution of (51) for some $j = 1, \ldots, n$. Because H has exactly $3n + 2$ eigenvalues and all of them are distinct (see lemma 4.1), all the solutions of the quadratic equation and of n cubic equations are multiplicity free and pairwise distinct.

Now the first part of theorem 5.1 follows from the remarks above, from (50) and lemma 2.1. Indeed if (50) admits a nontrivial solution for some λ_ν, then either $\lambda_\nu = 2\omega_2$ or

$$\mu = \big((\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_3) - (\lambda_\nu - 2\omega_3)D_1^2 - (\lambda_\nu - 2\omega_1)D_2^2 - (\lambda_\nu - 2\omega_2)D_3^2\big) \tag{63}$$

is an eigenvalue for $D_1\mathcal{D}_3\mathcal{D}_2^t + D_1\mathcal{D}_2\mathcal{D}_3^t$. The first case has been already discussed, while for the second we apply lemma 2.1. It follows then that μ is necessarily of the form

$$2D_1D_2D_3\cos\left(\frac{\pi j}{n+1}\right) \tag{64}$$

for some $j = 1, \ldots, n$. As was explained before, among those $3n$ eigenvalues constructed there are no repeated. The component $u_{(3)}$ of the corresponding eigenvectors are uniquely determined by the eigenvalues due to lemma 2.1. The other two components $u_{(1)}$ and $u_{(2)}$ are also uniquely determined by (46) and (47), respectively. This gives us a unique eigenvector u_ν of H for each solution of (51).

The second part of the statement follows from (34) because

$$\big(D_1\mathcal{D}_2^t + (\lambda_\nu - 2\omega_2)\mathcal{D}_3^t\big) \tag{65}$$

has rank n and its kernel is 0. □

6. Multiple-quantum spin dynamics of an inhomogeneous spin chain with $(3n + 2)$-sites

Information on the exact spectrum of the Hamiltonian of an open spin chain provides us with the techniques for determining the multi-quantum dynamics in such a system. The MQ NMR dynamics of the nuclear spins coupled by the nearest-neighbour dipolar interactions was developed in [2]. The corresponding Hamiltonian is

$$H_{\mathrm{MQ}} = \frac{1}{2}\sum_{n=1}^{N-1} D_{n,n+1}\{I_{n,+}I_{n+1,+} + I_{n,-}I_{n+1,-}\}. \tag{66}$$

The Hamiltonian H_{MQ} (66) is exactly of form (1) with the Larmor frequencies $\omega_n = 0$ for all the sites. The Liouville–von Neumann equation for the density matrix ρ ($\hbar = 1$)

$$\mathrm{i}\frac{\partial\rho}{\partial t} = [H_{\mathrm{MQ}}, \rho] \tag{67}$$

with the Hamiltonian H_{MQ} (66) gives us the intensities $G_n(t)$ of $n = 0$ and $n = \pm 2$ orders only, with the conservation conditions [13, 14]:

$$G_0(t) + G_2(t) + G_{-2}(t) = 1. \tag{68}$$

Theorem 6.1. *The intensities $G_n(t)$, $n = 0, \pm 2$, of MQ coherences of the Hamiltonian H_{MQ} (66) are*

$$G_0(t) = \frac{\mathrm{Tr}[\cos^2(D\cdot t)]}{N}, \qquad G_{\pm 2}(t) = \frac{\mathrm{Tr}[\sin^2(D\cdot t)]}{2N} \tag{69}$$

where D is defined in equation (2).

Proof. According to [10]

$$G_2(t) = G_{-2}(t) = \frac{1}{N} \sum_{k=1,3,\ldots} \sum_{n=2,4,\ldots} \left| \sum_{j=1}^{N} (-1)^j S_{jk} S_{jn}^* \right|^2, \tag{70}$$

with

$$S_{jk} = \sum_l u_{jl}^* u_{kl} \, \mathrm{e}^{-\frac{\mathrm{i}}{2}\lambda_l t}, \tag{71}$$

where λ_l are the eigenvalues of D, $l = 1, \ldots, N$, and the unitary matrix $U = \{u_{kl}\}_{k,l=1}^{N}$ diagonalizes D. Let us rewrite (70) in the matrix form

$$G_2(t) = G_{-2}(t) = \frac{1}{N} \operatorname{Tr}(B_0 A B_1 A^*), \tag{72}$$

where B_0 is the diagonal matrix with ones in odd rows and zeros in even rows, B_1 is the diagonal matrix with ones in even rows and zeros in odd rows:

$$B_0 = \operatorname{diag}\{1, 0, 1, 0, \ldots\}, \qquad B_1 = \operatorname{diag}\{0, 1, 0, 1, \ldots\};$$

and the matrix A is

$$A = S(B_1 - B_0)S^*, \qquad S = \exp\left(-\frac{\mathrm{i}}{2} D t\right). \tag{73}$$

Observe that

$$(B_1 - B_0)D = -D(B_1 - B_0). \tag{74}$$

Therefore,

$$(B_1 - B_0)S(B_1 - B_0) = S^* \qquad \text{and} \qquad \operatorname{Tr}[(S)^m] = \operatorname{Tr}[(S^*)^m]. \tag{75}$$

Using

$$A A^* = A^2 = I_N, \qquad A(B_1 - B_0)A^* = (B_1 - B_0)(S^*)^4 \tag{76}$$

and

$$\operatorname{Tr}[A(B_1 - B_0)A^*] = \operatorname{Tr}[(B_1 - B_0)A^* A] = \operatorname{Tr}[(B_1 - B_0)A A^*] \tag{77}$$

we deduce

$$\begin{aligned}
\operatorname{Tr}[B_0 A B_1 A^*] &= \frac{1}{4} \operatorname{Tr}[(I - (B_1 - B_0))A(I + (B_1 - B_0))A^*] \\
&= \frac{1}{4} \operatorname{Tr}[A A^* - (B_1 - B_0)A A^* + A(B_1 - B_0)A^* - (B_1 - B_0)A(B_1 - B_0)A^*] \\
&= \frac{1}{4} \operatorname{Tr}[I_N - (S^*)^4] = -\frac{1}{8} \operatorname{Tr}[S^4 + (S^*)^4 - 2I_N] \\
&= \frac{1}{2} \operatorname{Tr}\left[\left(\frac{S^2 - (S^*)^2}{2\mathrm{i}}\right)^2\right] = \frac{1}{2} \operatorname{Tr}[\sin^2(Dt)].
\end{aligned} \tag{78}$$

From here the result follows. □

Remark 6.1. In [7] formula (69) was proposed for alternating spin chains. Theorem 6.1 establishes the same formula for arbitrary spin chains coupled by the nearest-neighbour dipolar interactions.

Theorem 6.1 together with theorem 5.2 allows us to calculate MQ coherence intensities of the zero and the second orders, $G_0(t)$ and $G_2(t) + G_{-2}(t)$, without performing matrix

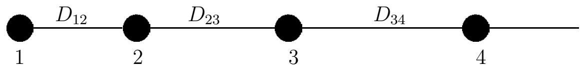

Figure 1. The four-spin fragment of the linear chain. The distances between neighbouring spins in the fragments are 2.7 Å, 3 Å and 3.3 Å. The dipolar coupling constants are $D_{12} = 2\pi \times 6096$, $D_{23} = 2\pi \times 4444$, $D_{34} = 2\pi \times 3339\,\text{s}^{-1}$.

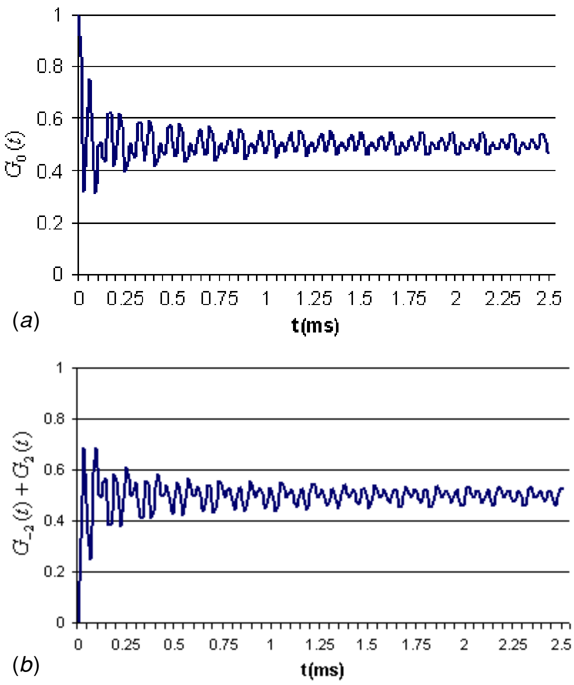

Figure 2. Time dependence of the intensity of MQ coherences of (*a*) the zeroth and (*b*) second order in a linear chain with 1001 spins coupled by the DDI among nearest neighbours. The linear chain consists of the fragments of figure 1 with the distances between neighbouring spins in the fragments 2.7 Å, 3 Å and 3.3 Å. The dipolar coupling constants are $D_{12} = 2\pi \times 6096$, $D_{23} = 2\pi \times 4444$, $D_{34} = 2\pi \times 3339$ s^{-1}.

multiplication, by solving $O(N)$ cubic equations (compare with [10]). Let us consider a linear spin chain of length 1001 which consists of four-spin fragments represented in figure 1.

The distances between neighbouring spins in the fragments are 2.7 Å, 3 Å and 3.3 Å. The dipolar coupling constants $D_{12} = 2\pi \times 6096$, $D_{23} = 2\pi \times 4444$ and $D_{34} = 2\pi \times 3339\,\text{s}^{-1}$ are used in all numerical calculations. The intensities of MQ coherences for the inhomogeneous linear chain with $N = 1001$ spins consisting of fragments of figure 1 are shown in figure 2. The dynamics behaviour coincides with that given in [10].

It is evident that the problem of diagonalization of the XY-Hamiltonian for open spin chains with periodic coupling constants is significantly more difficult than for cyclic systems [6]. However spin dynamics of open chains of coupling spins has some specific peculiarities which are different from dynamics of cyclic systems. The point is that dynamics of 1D systems has a spin-wave character. Spin-wave packets reflect at the ends of the chain [15]. Due to these effects in some cases spin dynamics of open 1D systems [15] is different from that of cyclic systems [16] even in systems with large numbers of spins and at long times. This explains our choice of the exact solution of the open linear spin chain model for the computation of the intensities of MQ coherences of the Hamiltonian H_{MQ} (66), which are experimentally measurable quantities describing spin dynamics of the open linear chains.

The above difference of open spin chains comparing with the cyclic systems makes open linear spin chains particularly useful for solving some problems of quantum information theory. As an example, we mention the problem of transferring qubits from the left end of the chain to its right end [8].

7. The generalization of the method for spin chains with $(kn-1)$-sites

Now we consider the case of a k-periodic system with $(kn-1)$-sites. According to section 3, to diagonalize Hamiltonian of such a system we have to solve the following system of linear equations:

$$\mathbf{H}\begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix} = \lambda_\nu \begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix}, \tag{79}$$

where

$$\mathbf{H} = \left[\begin{array}{ccccc|c} & & & & & \mathcal{D}_k^t \\ & & & & & 0 \\ & & \mathcal{H}_{1,k-1} & & & \vdots \\ & & & & & 0 \\ & & & & & \mathcal{D}_{k-1}^t \\ \mathcal{D}_k & 0 & \cdots & 0 & \mathcal{D}_{k-1} & 2\mathcal{W}_k \end{array}\right], \tag{80}$$

and

$$\mathcal{H}_{1,k-1} = \begin{bmatrix} 2\mathcal{W}_1 & \mathcal{D}_1 & 0 & \cdots & 0 & 0 \\ \mathcal{D}_1 & 2\mathcal{W}_2 & \mathcal{D}_2 & \cdots & 0 & 0 \\ 0 & \mathcal{D}_2 & 2\mathcal{W}_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2\mathcal{W}_{k-2} & \mathcal{D}_{k-2} \\ 0 & 0 & 0 & \cdots & \mathcal{D}_{k-2} & 2\mathcal{W}_{k-1} \end{bmatrix}. \tag{81}$$

Observe that because all $\mathcal{D}_j$, $j = 1, \ldots, k-2$, are diagonal $n \times n$ matrices, it is also true that

$$\mathcal{H}_{1,k-1} = H_{1,k-1} \otimes I_n. \tag{82}$$

Assume that λ_ν is not an eigenvalue for $\mathcal{H}_{1,k-1}$ (equivalently, is not an eigenvalue for $H_{1,k-1}$), and consider the matrix

$$\mathbf{G} = \left[\begin{array}{ccc|c} & & & 0 \\ & \left(\mathcal{H}_{1,k-1} - \lambda_\nu I_{n(k-2)}\right)^{-1} & & \vdots \\ & & & 0 \\ 0 & \cdots & 0 & I_{n-1} \end{array}\right]. \tag{83}$$

Under the above assumption on λ_ν the eigenvector equation

$$\mathbf{H}\begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix} = \lambda_\nu \begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix} \tag{84}$$

is equivalent to

$$\mathbf{G}\,(\mathbf{H}-\lambda_\nu I_{nk-1})\begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix} = 0, \tag{85}$$

or in another form to

$$\left[\begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 \\ \mathcal{D}_k & 0 & \cdots & 0 & \mathcal{D}_{k-1} \end{bmatrix} \mathbf{G} \begin{bmatrix} \mathcal{D}_k^t \\ 0 \\ \vdots \\ 0 \\ \mathcal{D}_{k-1}^t \\ 2\mathcal{W}_k - \lambda_\nu I_{n-1} \end{bmatrix}\right] \begin{bmatrix} u_{(1)} \\ u_{(2)} \\ \vdots \\ u_{(k-2)} \\ u_{(k-1)} \\ u_{(k)} \end{bmatrix} = 0. \tag{86}$$

Let us denote elements of the matrix $(H_{1,k-1} - \lambda_\nu I_{k-1})^{-1}$ by $P_{i,j}$ (where i is row, and j is column). Using

$$(\mathcal{H}_{1,k-1} - \lambda_\nu I_{n(k-1)})^{-1} = (H_{1,k-1} \otimes I_n - \lambda_\nu I_{k-1} \otimes I_n)^{-1} = (H_{1,k-1} - \lambda_\nu I_{k-1})^{-1} \otimes I_n,$$

we derive from (84) for $k-1 \geqslant j \geqslant 1$ that

$$u_{(j)} = -\big(P_{j,1}\mathcal{D}_k^t + P_{j,k-1}\mathcal{D}_{k-1}^t\big)u_{(k)}. \tag{87}$$

Substituting this expression with $j=1$ and $j=k-1$ into the last equation of (84) we obtain

$$\big(P_{1,1}\mathcal{D}_k\mathcal{D}_k^t + P_{1,k-1}\mathcal{D}_k\mathcal{D}_{k-1}^t + P_{k-1,1}\mathcal{D}_{k-1}\mathcal{D}_k^t + P_{k-1,k-1}\mathcal{D}_{k-1}\mathcal{D}_{k-1}^t\big)u_{(k)} = (2\omega_k - \lambda_\nu)u_{(k)}. \tag{88}$$

Because

$$\begin{aligned} \mathcal{D}_{k-1}\mathcal{D}_{k-1}^t &= D_{k-1}^2 I_{n-1}, & \mathcal{D}_k\mathcal{D}_k^t &= D_k^2 I_{n-1}, \\ \mathcal{D}_{k-1}\mathcal{D}_k^t &= D_{k-1}D_k J_{n-1}^t, & \mathcal{D}_k\mathcal{D}_{k-1}^t &= D_{k-1}D_k J_{n-1}, \end{aligned} \tag{89}$$

with the help of corollary 4.1 we derive that if λ_ν is not an eigenvalue of $H_{1,k-1}$, then the component $u_{(k)}$ of the corresponding eigenvector u_ν belongs to the kernel of

$$\begin{aligned} \mathcal{M} = (&\det(H_{2,k-1} - \lambda_\nu I_{k-2})D_k^2 + \det(H_{1,k-2} - \lambda_\nu I_{k-2})D_{k-1}^2 - (2\omega_k - \lambda_\nu) \\ &\times \det(H_{1,k-1} - \lambda_\nu I_{k-2}))I_{n-1} + (-1)^k D_1 \cdots D_k\big(J_{n-1} + J_{n-1}^t\big). \end{aligned} \tag{90}$$

Since

$$(2\omega_k - \lambda_\nu)\det(H_{1,k-1} - \lambda_\nu I_{k-2}) - \det(H_{1,k-2} - \lambda_\nu I_{k-2})D_{k-1}^2 = \det(H_{1,k} - \lambda_\nu I_k)$$

we can simplify the expression for $\mathcal{M}$:

$$\begin{aligned} \mathcal{M} = \big(&\det(H_{2,k-1} - \lambda_\nu I_{k-2})D_k^2 - \det(H_{1,k} - \lambda_\nu I_k)D_{k-1}^2\big)I_{n-1} \\ &+ (-1)^k D_1 \cdots D_k\big(J_{n-1} + J_{n-1}^t\big). \end{aligned} \tag{91}$$

Therefore,

$$\big(\det(H_{1,k} - \lambda_\nu I_k)D_{k-1}^2 - \det(H_{2,k-1} - \lambda_\nu I_{k-2})D_k^2\big)u_{(k)} = (-1)^k D_1 \cdots D_k\big(J_{n-1} + J_{n-1}^t\big)u_{(k)}. \tag{92}$$

We are ready to state the main result of the paper.

Theorem 7.1. *Each eigenvalue of the Hamiltonian H 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*

$$\det(H_{1,k}-\lambda_\nu I_k)-\det(H_{2,k-1}-\lambda_\nu I_{k-2})D_k^2=(-1)^k 2D_1\cdots D_k\cos\left(\frac{\pi j}{n}\right), \tag{93}$$

for some $j=1,\ldots,n-1$. Equation (93) does not have repeated roots and all $k(n-1)$ solutions constructed from (93) are pairwise distinct and are not eigenvalues for $H_{1,k-1}$.

If λ_ν is the solution of (93) for some $j=1,\ldots,n-1$, then it is an eigenvalue for H and the component $u_{(k)}$ of the corresponding eigenvector u_ν is

$$u_{(k)}=\left(\sin\left(\frac{\pi j}{n}\right),\ldots,\sin\left(\frac{(n-1)\pi j}{n}\right)\right). \tag{94}$$

The other components $u_{(j)}$, $j=1,\ldots,k-1$, are determined uniquely from

$$u_{(j)}=\frac{(-1)^{j-1}}{\det(H_{1,k-1}-\lambda_\nu I_{k-1})}\big[D_1\cdots D_{j-1}\det(H_{j+1,k-1}-\lambda_\nu I_{k-j-1})\mathcal{D}_k^t \\ +(-1)^{k-1}\det(H_{1,j-1}-\lambda_\nu I_{j-1})D_j\cdots D_{k-2}\mathcal{D}_{k-1}^t\big]u_{(k)}, \tag{95}$$

where $\mathcal{D}_{k-1},\mathcal{D}_k$ are given in (15) $(d=k-1)$. Every eigenvalue λ_ν of $H_{1,k-1}$ is an eigenvalue of H. The component $u_{(k)}$ of the corresponding eigenvector u_ν of H is zero. The component $u_{(1)}$ spans the one-dimensional kernel of

$$(-1)^{k-1}D_1\cdots D_{k-2}\mathcal{D}_{k-1}-\det(H_{2,k-1}-\lambda_\nu I_{k-2})\mathcal{D}_k. \tag{96}$$

The remaining components $u_{(j)}$, $j=2,\ldots,k-1$, are

$$u_{(j)}=(-1)^{j-1}\frac{D_1\cdots D_{j-1}\det(H_{j+1,k-1}-\lambda_\nu I_{k-j-1})}{\det(H_{2,k-1}-\lambda_\nu I_{k-2})}u_{(1)}. \tag{97}$$

Proof. The first part of the theorem follows from lemma 2.1 because H has exactly $(kn-1)$-distinct eigenvalues. Indeed, if an eigenvalue λ_ν of H is not an eigenvalue of $H_{1,k-1}$, then as was shown above, the component $u_{(k)}$ of the corresponding eigenvector u_ν of H satisfies (92). Therefore, λ_ν satisfies (93) for some $j=1,\ldots,n-1$.

For the second part of the theorem we again use lemma 2.1. The component $u_{(k)}$ of the corresponding eigenvector u_ν, satisfies (92), and, therefore, is uniquely determined by λ_ν as stated in lemma 2.1. The remaining components of the eigenvectors $u_{(\nu)}$ corresponding to the solutions of (93) can be reconstructed from (87) using corollary 4.3.

Finally, for the last part we observe that from lemma 4.2 and the property of the adjoint matrix

$$\begin{aligned}&D_{j-1}(-1)^{j-2}\frac{D_1\cdots D_{j-2}\det(H_{j,k-1}-\lambda_\nu I_{k-j})}{\det(H_{2,k-1}-\lambda_\nu I_{k-2})}\\ &\quad+(2\omega_j-\lambda_\nu)(-1)^{j-1}\frac{D_1\cdots D_{j-1}\det(H_{j+1,k-1}-\lambda_\nu I_{k-j-1})}{\det(H_{2,k-1}-\lambda_\nu I_{k-2})}\\ &\quad+D_j(-1)^j\frac{D_1\cdots D_j\det(H_{j+2,k-1}-\lambda_\nu I_{k-j-2})}{\det(H_{2,k-1}-\lambda_\nu I_{k-2})}\\ &=D_{j-1}\frac{\mathrm{adj}_{1,j-1}\{(\mathrm{H}_{1,k-1}-\lambda_\nu\mathrm{I}_{k-1})\}}{\det(H_{2,k-1}-\lambda_\nu I_{k-2})}+(2\omega_j-\lambda_\nu)\frac{\mathrm{adj}_{1,j}\{(\mathrm{H}_{1,k-1}-\lambda_\nu\mathrm{I}_{k-1})\}}{\det(H_{2,k-1}-\lambda_\nu I_{k-2})}\\ &\quad+D_j\frac{\mathrm{adj}_{1,j+1}\{(\mathrm{H}_{1,k-1}-\lambda_\nu\mathrm{I}_{k-1})\}}{\det(H_{2,k-1}-\lambda_\nu I_{k-2})}\\ &=\delta_{1,j}\frac{\det(H_{1,k-1}-\lambda_\nu I_{k-1})}{\det(H_{2,k-1}-\lambda_\nu I_{k-2})}=0,\end{aligned} \tag{98}$$

where $k-1>j>1$ and $\delta_{i,j}$ is the Kronecker symbol. We also have

$$D_{k-2}(-1)^{k-3}\frac{D_1\cdots D_{k-3}(2\omega_{k-1}-\lambda_\nu)}{\det(H_{2,k-1}-\lambda_\nu I_{k-2})}+(2\omega_{k-1}-\lambda_\nu)(-1)^{k-2}\frac{D_1\cdots D_{k-2}}{\det(H_{2,k-1}-\lambda_\nu I_{k-2})}=0. \tag{99}$$

If λ_ν is an eigenvalue for $H_{1,k-1}$, then

$$2\omega_1+D_1(-1)\frac{D_1\det(H_{3,k-1}-\lambda_\nu I_{k-2})}{\det(H_{2,k-1}-\lambda_\nu I_{k-2})}=\frac{\det(H_{1,k-1}-\lambda_\nu I_{k-2})}{\det(H_{2,k-1}-\lambda_\nu I_{k-2})}=0. \tag{100}$$

Therefore, if $u_{(1)}$ spans the kernel of

$$(-1)^{k-1}D_1\cdots D_{k-2}\mathcal{D}_{k-1}-\det(H_{2,k-1}-\lambda_\nu I_{k-2})\mathcal{D}_k \tag{101}$$

and $u_{(k)}=0$, then vector u_ν with the other components given by (97) does satisfy the eigenvalue equation

$$(H-\lambda I_{kn-1})u_\nu=0. \tag{102}$$

This completes the proof. □

8. Conclusion

In this paper, we proposed a new one-dimensional exactly solvable model for a linear k-periodic (in space) open spin chain with $(kn-1)$-sites. For the diagonalization procedure it is important that the number of sites is $(k-1)(\mathrm{mod}\, k)$. Nevertheless, the model can serve as a good approximation for any open linear periodic spin system if the number of sites in it is much more than the period.

The developed method of diagonalization of the XY-Hamiltonian of inhomogeneous linear spin chains can be applied to different problems of quantum information theory [3, 7, 8] and spin dynamics. This method allows us to avoid matrix multiplications which are time-consuming operations in the systems with large numbers of spins. In some cases we can suggest analytical methods for problems of spin dynamics instead of the known numerical ones [9].

The proposed method of diagonalization could also be applied to different physical and technical problems which use three-diagonal matrices [18]. In particular, new numerical methods of solving such problems could be worked out on the basis of the approach proposed in this paper, and further factorizations of multivariable hypergeometric series for some eigenvalues of general tridiagonal matrices [17] could be obtained.

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