The Hilbert Space and the Exact Solution of the Spin-Electron Double-Tetrahedral Chain

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We discuss an exactly solvable double-tetrahedral chain, in which the localized Ising spins regularly alternate with triangular clusters — each available for one mobile electron. We give an exact solution for the considered hybrid system by the construction of the N -th tensor power of the Fourier transformation and using the generalized decoration-iteration mapping transformation.

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1. Introduction

One-dimensional (1D) discrete dynamical systems are intensively studied by both theorists and experimentalists mainly due to their possible applications in intensively studied carbon nanotubes [1], 1D organic superconductors [2], as well as 1D organic ferromagnets [3]. There is also a possibility of designing 1D models of fermionic quantum gas loaded into an optical lattice [4], which is a promising candidate for quantum information processing.

In this work, we will consider a hybrid magnetic system on a double-tetrahedral chain in an external magnetic field, where N nodal lattice sites occupied by the localized Ising spins regularly alternate with triangular clusters with the dynamics described by the Hubbard Hamiltonian [5].

2. Hamiltonian and Hilbert space

The Hamiltonian of the considered 1D magnetic system can be expressed as a sum over N block Hamiltonians H_k that contain the one triangular cluster and its nearest-neighbouring nodal lattice sites (see Fig. 1):

$$H = \sum_{k=1}^N H_k, \quad (1)$$

$$\begin{aligned} H_k = & -t \sum_{\alpha \in \{\uparrow, \downarrow\}} \sum_{j \in \tilde{3}} (c_{kj, \alpha}^\dagger c_{kj+1, \alpha} + c_{kj+1, \alpha}^\dagger c_{kj, \alpha}) \\ & + \frac{J}{2} (\sigma_k^z + \sigma_{k+1}^z) \sum_{j \in \tilde{3}} (n_{kj, \uparrow} - n_{kj, \downarrow}) \\ & - \frac{H_I}{2} (\sigma_k^z + \sigma_{k+1}^z) - \frac{H_e}{2} \sum_{j \in \tilde{3}} (n_{kj, \uparrow} - n_{kj, \downarrow}). \end{aligned} \quad (2)$$

Fig. 1. A part of the spin-electron system on tetrahedral chain. The white (black) circles indicate the lattice sites available for localized Ising spins (mobile electrons).

Above, the periodic boundary condition $c_{k4, \alpha}^\dagger = c_{k1, \alpha}^\dagger$ ($c_{k4, \alpha} = c_{k1, \alpha}$) is assumed, $\tilde{3} = \{1, 2, 3\}$ represents the set of lattice sites forming triangular clusters, $c_{kj, \alpha}^\dagger$ ($c_{kj, \alpha}$) is the usual fermionic creation (annihilation) operator for mobile electrons with the spin $\alpha = \{\uparrow, \downarrow\}$, $n_{kj, \alpha} = c_{kj, \alpha}^\dagger c_{kj, \alpha}$ labels the respective number operator and $\sigma_k^z = \pm 1/2$ stands for the Ising spins. The parameter $t > 0$ takes into account the kinetic energy of a single mobile electron delocalized over the triangular cluster and J denotes the Ising exchange interaction between electrons and their nearest Ising neighbours. Finally, H_I and H_e are the Zeeman terms acting on the localized Ising spins and mobile electrons, respectively.

The considered model may be alternatively viewed as a set of N tetrahedrons with one vertex occupied by the localized Ising spin and three vertices available for one mobile electron on a fictitious 1D linear chain. From this perspective the Hilbert space $\mathcal{H}$ of the system can be created by defining the *block space* h_k with the basis consisting of eigenvectors that denote all possible occupations of all magnetic particles from k -th tetrahedron

$$h_k = h_I \otimes h_e, \quad (3)$$

where h_I represents the *1-site subspace* spanned over two possible projections of the localized Ising spin,

$$h_I = \text{lc}_{\mathbb{C}}\{\uparrow, \downarrow\}, \quad \dim h_I = 2, \quad (4)$$

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and h_e represents the 3-sites subspace spanned over the orthonormal basis of the electron states:

$$h_e = l_{\mathbb{C}}\{c_{k1,\uparrow}^\dagger|0\rangle, c_{k2,\uparrow}^\dagger|0\rangle, c_{k3,\uparrow}^\dagger|0\rangle,$$

$$c_{k1,\downarrow}^\dagger|0\rangle, c_{k2,\downarrow}^\dagger|0\rangle, c_{k3,\downarrow}^\dagger|0\rangle\}, \quad \dim h_e = 6. \quad (5)$$

Here, the symbol $l_{\mathbb{C}}A$ stands for the linear closure of a set A over the complex field $\mathbb{C}$ and $|0\rangle$ denotes the vacuum state. Due to the obvious translational symmetry of triangular clusters available for mobile electrons ($c_{k4,\alpha}^\dagger = c_{k1,\alpha}^\dagger$, $c_{k4,\alpha} = c_{k1,\alpha}$), the basis of electron states (5) can be divided into two orbits of the cyclic group C_3 with opposite electron configurations $\alpha = \uparrow, \downarrow$:

$$\mathcal{O}_\alpha = \{|f_{k1}\rangle = c_{k1,\alpha}^\dagger|0\rangle, |f_{k2}\rangle =$$

$$c_{k2,\alpha}^\dagger|0\rangle, |f_{k3}\rangle = c_{k3,\alpha}^\dagger|0\rangle\}. \quad (6)$$

The symbol $|f_{kj}\rangle$ in Eq. (6) denotes the mobile electron configuration at the j -th lattice site of the k -th triangular cluster. The mobile electron configuration f_{k1} for $j = 1$ is called the *initial mobile electron configuration*. In view of this notation, the block space h_k given by Eq. (3) can be expressed as

$$h_k = l_{\mathbb{C}}\{|\sigma_k \otimes f_{kj}\rangle \equiv |\sigma_k, f_{kj}\rangle | j \in \tilde{3}\}. \quad (7)$$

Finally, the Hilbert space $\mathcal{H}$ of all quantum states of the investigated spin-electron system on double-tetrahedral chain can be obtained in the form

$$\mathcal{H} = \prod_{k=1}^N \otimes h_k. \quad (8)$$

3. Eigenvalues and eigenvectors

Owing to the definition of the investigated spin-electron model, the block Hamiltonian (2) commutes with the z -th component of the total spin operator $S_k^z = \sum_{j \in \tilde{3}} (n_{kj,\uparrow} - n_{kj,\downarrow})/2 = \pm 1/2$ for one electron from k -th triangular cluster. Consequently, the up- and down-spin configurations of the mobile electron from k -th triangular cluster are separately conserved. As a result, the matrix representation of the block Hamiltonian (2) splits into two matrix sectors $H(S_k^z)$ corresponding to the orbits (6) with opposite electron configurations

$$H_k(\pm 1/2) = \begin{pmatrix} \pm h'_e - h'_I & -t & -t \\ -t & \pm h'_e - h'_I & -t \\ -t & -t & \pm h'_e - h'_I \end{pmatrix}. \quad (9)$$

Above, we have introduced the notation $h'_e = J(\sigma_k + \sigma_{k+1})/2 - H_e/2$, $h'_I = H_I(\sigma_k + \sigma_{k+1})/2$ in order to write the matrices (9) in a more abbreviated form. The matrix sectors (9) can be completely diagonalized in one step by using the co-called *basis of wavelets* [6–8], i.e. the discrete Fourier transformation of the orbits (6) of the group C_3 , as the aftermath of the translational symmetry of a fictitious 1D linear chain of the triangular clusters. The appropriate amplitude takes the form

$$|\kappa_k\rangle = \frac{1}{\sqrt{3}} \sum_{j \in \tilde{3}} \exp(i2\pi\kappa_k j/3) |f_{kj}\rangle, \quad (10)$$

where $i = \sqrt{-1}$ and the quasi-momentum κ_k takes the values from the Brillouin zone $B = \{\kappa_k = 0, \pm 1\}$. The matrix sectors (9) in the basis of wavelets take the following diagonal form:

$$H_k(\pm 1/2) =$$

$$\begin{pmatrix} \pm h'_e - h'_I - 2t & 0 & 0 \\ 0 & \pm h'_e - h'_I + t & 0 \\ 0 & 0 & \pm h'_e - h'_I + t \end{pmatrix}, \quad (11)$$

which straightforwardly show a complete set of the eigenvalues for the block Hamiltonian (2) in the relevant Hilbert subspaces

$$E_{k1,k2} = h'_e - h'_I + t, \quad E_{k4,k5} = -h'_e - h'_I + t,$$

$$E_{k3} = h'_e - h'_I - 2t, \quad E_{k6} = -h'_e - h'_I - 2t. \quad (12)$$

It is noteworthy that the all eigenvalues E_{km} depend on the values of the Ising spins σ_k and σ_{k+1} through the parameters h'_e and h'_I .

The appropriate eigenvectors can also be obtained by the irreducible basis of the cyclic group C_3 forming the N -th tensor power of a discrete Fourier transformation

$$|\kappa_1, \kappa_2, \dots, \kappa_N\rangle =$$

$$\prod_{k=1}^N \otimes \frac{1}{\sqrt{3}} \sum_{j \in \tilde{3}} \exp(i2\pi\kappa_k j/3) |\sigma_k, f_{kj}\rangle. \quad (13)$$

For $\kappa_1 = \kappa_2 = \dots = \kappa_N = 0$ the eigenvectors (13) may constitute the ferromagnetic or antiferromagnetic ground states with the spin-electron configurations $(\sigma_k, \alpha) = (\uparrow, \uparrow)$ and $(\sigma_k, \alpha) \in \{(\uparrow, \downarrow), (\downarrow, \uparrow)\}$, respectively, due to a mutual interplay between the interaction parameters J and t as well as the magnetic fields H_e , H_I applied on the magnetic particles of the system (for more details see Ref. [5]).

4. Partition function

Next, according to the magnetic structure shown in Fig. 1, the spin-electron double-tetrahedral chain may be classified to a class of bond-decorated Ising models, whose partition function can be exactly derived using the generalized decoration-iteration transformation (DIT) technique [9]. Actually, with regard to the commuting character of the block Hamiltonians H_k ($[H_k, H_l] = 0$, where $k \neq l$), the partition function Z of the considered system can be partially factorized into a product of cluster partition functions Z_k :

$$Z = \sum_{\{\sigma_j\}} \prod_{k=1}^N \text{Tr}_k \exp(-\beta H_k) = \sum_{\{\sigma_j\}} \prod_{k=1}^N Z_k. \quad (14)$$

Above, $\beta = 1/(k_B T)$, k_B is the Boltzmann constant, T is the temperature, $\sum_{\{\sigma_j\}}$ denotes a summation over all possible states of the localized Ising spins and Tr_k labels a trace over degrees of freedom of mobile electron from the k -th triangular cluster. The cluster partition function Z_k can be easily obtained by using a set of eigenvalues E_{km} corresponding to the block Hamiltonian H_k listed in Eq. (12):

$$Z_k = \sum_{m=1}^6 \exp(-\beta E_{km}) = 2 \exp(\beta h'_I) [2 \exp(-\beta t) + \exp(2\beta t)] \cosh(\beta h'_e). \quad (15)$$

The above resulting expression of the cluster partition function Z_k immediately implies a possibility of performing the generalized DIT

$$Z_k = A \exp[\beta J_{\text{eff}} \sigma_k \sigma_{k+1} + \beta H_{\text{eff}} (\sigma_k + \sigma_{k+1})/2], \quad (16)$$

which, from the physical point of view, removes all the interaction parameters associated with a triangular cluster available for mobile electron from the k -th block and replaces them by the effective exchange interaction J_{eff} and the effective external field H_{eff} acting on the remaining Ising spins localized at k -th and $(k+1)$ -th nodal lattice sites. In this way, one finds a simple connection between the studied spin-electron double-tetrahedral chain and the uniform spin-1/2 Ising chain with the effective nearest-neighbour interaction J_{eff} and the effective field H_{eff} . Of course, the transformation relation (13) must hold for all possible spin combinations of the Ising spins σ_k, σ_{k+1} . This *self-consistency condition* unambiguously determines mapping parameters A, J_{eff} and H_{eff} :

$$A = 2 [2 \exp(-\beta t) + \exp(2\beta t)] (V_- V_+ V^2)^{1/4},$$

$$J_{\text{eff}} = T \ln \left(\frac{V_- V_+}{V^2} \right), \quad H_{\text{eff}} = H_I + T \ln \left(\frac{V_-}{V_+} \right), \quad (17)$$

where $V_{\mp} = \cosh(\beta J/2 \mp \beta H_e/2)$ and $V = \cosh(\beta H_e/2)$. Finally, a direct substitution of the transformation relation (16) into Eq. (14) yields the equality

$$Z = A^N Z_I, \quad (18)$$

which introduces an exact mapping relationship between the partition function Z of the studied spin-electron double-tetrahedral chain and the partition function Z_I of the uniform spin-1/2 Ising linear chain with the nearest-neighbour coupling J_{eff} and the magnetic field H_{eff} . The mapping relation (18) in fact completes the exact evaluation of the partition function, since the partition function of the uniform spin-1/2 Ising chain is well known [10].

5. Conclusions

In this paper, the hybrid spin-electron system in an external magnetic field on the 1D double-tetrahedral chain, in which the localized Ising spins regularly alternate with triangular clusters available for one mobile electron has been considered. We gave the detailed analysis of the cluster space h_k using the representation group theory of the cyclic group C_3 . Next, we constructed the N -th tensor power of the discrete Fourier transformation, which provides the eigenvalues and eigenvectors of the spin-electron system. Finally, by using the decoration-iteration mapping approach, we introduced the procedure of the exact solution of the partition function for the considered system, which can readily be utilized for calculation of all important physical quantities

(magnetization, entropy, specific heat, susceptibility) by utilizing the standard thermodynamical-statistical relations. Generalization of the obtained exact results to the spin-electron system, in which triangular clusters are available for more than one mobile electron, is still the open question and constitutes the main topics of our research in the near future.

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