



On the quantum correlations in two-qubit XYZ spin chains with Dzyaloshinsky–Moriya and Kaplan–Shekhtman–Entin-Wohlman–Aharony interactions

M. A. Yurischev¹

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Abstract

The anisotropic Heisenberg two-spin-1/2 model in an inhomogeneous magnetic field with both antisymmetric Dzyaloshinsky–Moriya and symmetric Kaplan–Shekhtman–Entin-Wohlman–Aharony cross interactions is considered at thermal equilibrium. Using a group-theoretical approach, we find fifteen spin Hamiltonians and as many corresponding Gibbs density matrices (quantum states) whose eigenvalues are expressed only through square radicals. We also found local unitary transformations that connect nine of this fifteen state collection, and one of them is the X quantum state. Since such quantum correlations as quantum entanglement, quantum discord, one-way quantum work deficit, and others are known for the X state, this allows to get the quantum correlations for any member from the nine state family. Further, we show that the remaining six quantum states are separable and that they are also connected by local unitary transformations, but, however, now the case with known correlations beyond entanglement is generally not available.

Keywords Quantum correlation theory · Group-theoretical analysis · Local unitary transformations · X density matrix · Non-X quantum states

1 Introduction

To explain the phenomenon of weak ferromagnetism observed in some rhombohedral antiferromagnets, Dzyaloshinsky [1,2] developed a phenomenological approach based on the Landau theory of second-order phase transitions and showed that the *antisymmetric* mixed (in magnetization components) term in the expansion of the thermodynamic potential is responsible for the appearance of nonzero net magnetiza-

✉ M. A. Yurischev
yur@itp.ac.ru

¹ Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, 142432 Moscow Region, Russia

tion of the system. Shortly after [3], he also noticed that in antiferromagnetic crystals with the tetragonal lattices, weak ferromagnetism can be caused by the *symmetric* mixed term in the expansion of the corresponding thermodynamic potential.

Later on, in 1960, Moriya [4,5] developed a microscopic theory of anisotropic superexchange interaction by extending the Anderson theory of superexchange to include spin–orbit coupling. Using perturbation theory, he found that the leading anisotropy contribution to the interaction between two neighboring spins σ_1 and σ_2 is given by

$$\mathcal{H}_{\text{DM}} = \mathbf{D} \cdot (\sigma_1 \times \sigma_2), \quad (1)$$

where $\mathbf{D} = (D_x, D_y, D_z)$ is a constant vector that characterizes a substance. This interaction reproduces Dzyaloshinsky’s antisymmetric term and is now referred to as the Dzyaloshinsky–Moriya (DM) interaction. In addition, Moriya found the second-order correction term [4,5]

$$\mathcal{H}_{\text{KSEA}} = \sigma_1 \cdot \tilde{\Gamma} \cdot \sigma_2, \quad (2)$$

where $\tilde{\Gamma}$ is a symmetric traceless tensor. For a long time, this interaction was assumed to be negligible compared with the antisymmetric contribution (1). However, more later Kaplan [6] and then Shekhtman et al. [7,8] argued the importance of the symmetric term because it can restore the $O(3)$ invariance of the isotropic Heisenberg system which is broken by the DM term. For this reason, the interaction (2) began to be called the Kaplan–Shekhtman–Entin-Wohlman–Aharony (KSEA) interaction [9,10] (see also reference 14 in [11]).

We will discuss two-site systems with the Hamiltonian

$$\mathcal{H} = \mathcal{H}_Z + \mathcal{H}_H + \mathcal{H}_{\text{DM}} + \mathcal{H}_{\text{KSEA}}, \quad (3)$$

where \mathcal{H}_Z is the Zeeman energy and \mathcal{H}_H the anisotropic exchange Heisenberg interactions. Behavior of quantum correlations in different particular cases of the model (3) was considered in numerous papers. The behavior of thermal entanglement in two-qubit completely isotropic (XXX) Heisenberg chain in the absence of an external field, but in the presence of DM interaction with a nonzero of only one, D_z , component of the Dzyaloshinsky vector \mathbf{D} was considered in [12]. The author of this paper found that the DM interaction can excite entanglement. Thermal entanglement in the partially anisotropic (XXZ) Heisenberg model with D_z or D_x component of Dzyaloshinsky vector was studied in [13]. Quantum entanglement in anisotropic Heisenberg XXZ chain with only D_z component was also discussed in [14]. The authors established that while the anisotropy suppresses the entanglement, the DM interaction can restore it. The effect of DM interaction on the quantum entanglement in the Heisenberg XYZ chain was observed in [15] in the absence of magnetic field. Thermal quantum discord in the anisotropic Heisenberg XXZ model with DM interaction and without any external field was investigated in [16]. Concurrence and quantum discord in two-qubit anisotropic Heisenberg XXZ model with DM interaction along the z -direction was considered in [17] where it was found that the tunable parameter D_z may play a constructive role to the quantum correlations in thermal equilibrium. Quantum discord of two-qubit anisotropy XXZ Heisenberg chain with DM interaction under uniform magnetic field was investigated in [18]. In the recent papers [19,20], the thermal quantum

entanglement and discord in two-qubit XYZ chain with DM interaction were discussed. As a whole, one can conclude that the most results have been obtained for the spin pairs with DM interactions when the exchange Heisenberg couplings are isotropic or, rarer, anisotropic. The external magnetic field was taken into account much less frequently. Finally, there are no publications where the quantum correlations (entanglement, discord, etc.) in Heisenberg dimers were discussed in the presence of KSEA interactions. Our research fills these gaps to a certain extent.

The structure of this paper is as follows. In the next section, we write down the Hamiltonian in an expanded form and establish its relationship with the density matrix. Sections 3 and 4 deal with the X and CS quantum states what gives the key that opens the way, first, to the group-theoretical analysis in Sect. 5 and then, in Sect. 6, to the results for the D_y and Γ_y pair components of Dzyaloshinsky vector and $\hat{\Gamma}$ tensor. Section 7 is devoted to the classification of fifteen Hamiltonians and density matrices. Finally, in the last Sect. 8, we briefly summarize the results obtained and note the remaining unsolved problems.

2 Hamiltonian and density matrix

The DM interaction (1) can be written in an expanded form as

$$\mathbf{D} \cdot (\boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2) = D_x(\sigma_1^y \sigma_2^z - \sigma_1^z \sigma_2^y) + D_y(\sigma_1^z \sigma_2^x - \sigma_1^x \sigma_2^z) + D_z(\sigma_1^x \sigma_2^y - \sigma_1^y \sigma_2^x), \quad (4)$$

where $\boldsymbol{\sigma}_i$ denotes the vector of Pauli matrices at site $i = 1, 2$; $\boldsymbol{\sigma}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$. Similarly for the KSEA term (2):

$$\begin{aligned} \boldsymbol{\sigma}_1 \cdot \tilde{\Gamma} \cdot \boldsymbol{\sigma}_2 &= (\sigma_1^x, \sigma_1^y, \sigma_1^z) \begin{pmatrix} 0 & \Gamma_z & \Gamma_y \\ \Gamma_z & 0 & \Gamma_x \\ \Gamma_y & \Gamma_x & 0 \end{pmatrix} \begin{pmatrix} \sigma_2^x \\ \sigma_2^y \\ \sigma_2^z \end{pmatrix} \\ &= \Gamma_x(\sigma_1^y \sigma_2^z + \sigma_1^z \sigma_2^y) + \Gamma_y(\sigma_1^z \sigma_2^x + \sigma_1^x \sigma_2^z) + \Gamma_z(\sigma_1^x \sigma_2^y + \sigma_1^y \sigma_2^x), \quad (5) \end{aligned}$$

where $\Gamma_x, \Gamma_y,$ and Γ_z are the elements of the tensor $\tilde{\Gamma}$. As a result, the Hamiltonian (3) is rewritten as

$$\begin{aligned} \mathcal{H} &= B_1^x \sigma_1^x + B_1^y \sigma_1^y + B_1^z \sigma_1^z + B_2^x \sigma_2^x + B_2^y \sigma_2^y + B_2^z \sigma_2^z \\ &+ J_x \sigma_1^x \sigma_2^x + J_y \sigma_1^y \sigma_2^y + J_z \sigma_1^z \sigma_2^z \\ &+ D_x(\sigma_1^y \sigma_2^z - \sigma_1^z \sigma_2^y) + D_y(\sigma_1^z \sigma_2^x - \sigma_1^x \sigma_2^z) + D_z(\sigma_1^x \sigma_2^y - \sigma_1^y \sigma_2^x) \\ &+ \Gamma_x(\sigma_1^y \sigma_2^z + \sigma_1^z \sigma_2^y) + \Gamma_y(\sigma_1^z \sigma_2^x + \sigma_1^x \sigma_2^z) + \Gamma_z(\sigma_1^x \sigma_2^y + \sigma_1^y \sigma_2^x), \quad (6) \end{aligned}$$

where B_i^α ($i = 1, 2; \alpha = x, y, z$) are the components of the external magnetic fields \mathbf{B}_1 and \mathbf{B}_2 (with the incorporated gyromagnetic ratios or g -factors) and J_α ($\alpha = x, y, z$) are the Heisenberg exchange couplings.

We will be able to study the systems only in some special cases of the Hamiltonian (6). For them, we will be interested in systems in a state of thermal equilibrium.

The corresponding Gibbs density matrix is given as

$$\rho = \frac{1}{Z} \exp(-\mathcal{H}/T), \tag{7}$$

where T is the temperature in energy units and Z the partition function. Thus, the Hamiltonian and density matrix of any system are connected via the functional relation.

Quantum correlations contained in composite quantum states are the focus of quantum information science. Many measures have been proposed to quantify these correlations, such as quantum entanglement, quantum discord, and one-way quantum work deficit [21–28]. It should be emphasized that the quantum correlation measures must satisfy a number of criteria [29] (see also the review [24]). In particular, as a necessary condition, the measures must be invariant under any *local* unitary transformations.

3 XYZ chain with D_z and Γ_z couplings

We begin the analysis with quantum states having the X form. In accord with definition, X matrix can have nonzero entries only on the main diagonal and anti-diagonal. The portrait of such a sparse matrix resembles the letter “X,” which allowed to give it such a name [30]. Algebraic characterization of X states in quantum information has been done by Rau [31]. It is important to note that both the sums and the products of X matrices are again the X matrices; that is, the set of X matrices is algebraically closed. In particular, a function (decomposable in a Taylor series) of X matrix is the X matrix.

In the most general form, the Hermitian X matrix corresponding to the Hamiltonian (6) can be written as

$$\mathcal{H}_{zz} = \begin{pmatrix} J_z + B_1^z + B_2^z & \cdot & \cdot & J_x - J_y - 2i\Gamma_z \\ \cdot & -J_z + B_1^z - B_2^z & J_x + J_y + 2iD_z & \cdot \\ \cdot & J_x + J_y - 2iD_z & -J_z - B_1^z + B_2^z & \cdot \\ J_x - J_y + 2i\Gamma_z & \cdot & \cdot & J_z - B_1^z - B_2^z \end{pmatrix}, \tag{8}$$

where the points are put instead of zero entries. In Eq.(8), B_1^z and B_2^z are the z -components of external fields applied at the 1st and 2nd qubits, respectively, (J_x, J_y, J_z) the vector of interaction constants of the Heisenberg part of interaction, D_z the z -component of Dzyaloshinsky vector, and Γ_z the z -component in the KSEA interaction. Thus, this model contains seven real independent parameters: $B_1^z, B_2^z, J_x, J_y, J_z, D_z,$ and Γ_z .

On the other hand, “any four-by-four matrix—and, therefore, the Hamiltonian matrix in particular—can be written as a linear combination of the sixteen double-spin matrices” [32, Sect. 12-2]. For the traceless X matrix (8), the linear combination of “double-spin matrices” is given as

$$\mathcal{H}_{zz} = B_1^z \sigma_1^z + B_2^z \sigma_2^z + J_x \sigma_1^x \sigma_2^x + J_y \sigma_1^y \sigma_2^y + J_z \sigma_1^z \sigma_2^z + J_{xy} \sigma_1^x \sigma_2^y + J_{yx} \sigma_1^y \sigma_2^x, \tag{9}$$

where

$$J_{xy} = D_z + \Gamma_z, \quad J_{yx} = -D_z + \Gamma_z. \tag{10}$$

Due to the functional relation (7), the Gibbs density matrix also has the X form with seven real parameters:

$$\begin{aligned} \rho_{zz} = & \begin{pmatrix} a & \cdot & \cdot & u \\ \cdot & b & v & \cdot \\ \cdot & v^* & c & \cdot \\ u^* & \cdot & \cdot & d \end{pmatrix} = \frac{1}{4}(\sigma_0 \otimes \sigma_0 + s_1^z \sigma_z \otimes \sigma_0 + s_2^z \sigma_0 \otimes \sigma_z \\ & + c_1 \sigma_x \otimes \sigma_x + c_2 \sigma_y \otimes \sigma_y + c_3 \sigma_z \otimes \sigma_z + c_{12} \sigma_x \otimes \sigma_y + c_{21} \sigma_y \otimes \sigma_x), \end{aligned} \tag{11}$$

where the asterisk denotes complex conjugation, $s_1^z, s_2^z, c_1, c_2, c_3, c_{12}$, and c_{21} are the unary and binary correlation functions, and

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{12}$$

are the unit and Pauli spin operators in the standard representation. Due to the nonnegativity definition and normalization condition of any density operator, $a, b, c, d \geq 0$, $a + b + c + d = 1$, $ad \geq |u|^2$, and $bc \geq |v|^2$.

One can now calculate different quantum correlations in the X quantum states. The methods of calculating quantum correlations for the two-qubit X quantum states have been developed in a number works. The concurrence, a measure of quantum entanglement, is given by [30]

$$C = 2 \max \left\{ 0, |u| - \sqrt{bc}, |v| - \sqrt{ad} \right\}. \tag{13}$$

There are considerable studies on the quantum discord and one-way quantum work deficit. For instance, the quantum discord of two-qubit X quantum states was considered in Refs. [33–35] (and references therein). One may present the quantum discord as a formula

$$Q = \min\{Q_0, Q_{\tilde{\theta}}, Q_{\pi/2}\}, \tag{14}$$

where the subfunctions (branches) Q_0 and $Q_{\pi/2}$ are the analytical expressions (corresponding to the discord with optimal measurement angles 0 and $\pi/2$, respectively) and only the third branch $Q_{\tilde{\theta}}$ requires one-dimensional searching of the optimal state-dependent measurement angle $\tilde{\theta} \in (0, \pi/2)$ (for details see in Refs. [36–39]).

Very similar situation takes place for the one-way quantum work deficit [40–42]. We may again write the one-way quantum work deficit of two-qubit X state in a semi-analytical form:

$$\Delta = \min\{\Delta_0, \Delta_{\vartheta}, \Delta_{\pi/2}\}, \tag{15}$$

where the branches Δ_0 and $\Delta_{\pi/2}$ are known in the analytical form, while the third branch Δ_{ϑ} also requires to perform numerical minimization to obtain state-dependent minimizing polar angle $\vartheta \in (0, \pi/2)$ (see [42–45]).

So, the theory to calculate quantum correlations of X quantum states is well developed. This gives a possibility to calculate and investigate different quantum correlations for the two-qubit systems in a nonuniform field in z -direction, with completely anisotropic Heisenberg interactions, and with arbitrary z -components of DM and KSEA interactions.

4 XYZ chain with D_x and Γ_x couplings

Let us take the centrosymmetric (CS) quantum state now. The CS matrix $n \times n$ is defined by the relations for its matrix elements as follows: $a_{ij} = a_{n+1-i, n+1-j}$ [46]. It is easy to check that the sum and product of CS matrices are the CS matrix, i.e., this family of matrices as well as X matrices is algebraically closed.

Most general Hermitian CS matrix of fourth order looks as

$$\rho_{xx} = \begin{pmatrix} a & \mu & \nu & c \\ \mu^* & b & d & \nu^* \\ \nu^* & d & b & \mu^* \\ c & \nu & \mu & a \end{pmatrix}, \quad (16)$$

where $a, b, c,$ and d are real quantities, while μ and ν are complex.

The Hamiltonian with CS symmetry reads

$$\mathcal{H}_{xx} = \begin{pmatrix} J_z & B_2^x - iJ_{zy} & B_1^x - iJ_{yz} & J_x - J_y \\ B_2^x + iJ_{zy} & -J_z & J_x + J_y & B_1^x + iJ_{yz} \\ B_1^x + iJ_{yz} & J_x + J_y & -J_z & B_2^x + iJ_{zy} \\ J_x - J_y & B_1^x - iJ_{yz} & B_2^x - iJ_{zy} & J_z \end{pmatrix}. \quad (17)$$

This Hamiltonian in the Bloch form is written as

$$\mathcal{H}_{xx} = B_1^x \sigma_1^x + B_2^x \sigma_2^x + J_x \sigma_1^x \sigma_2^x + J_y \sigma_1^y \sigma_2^y + J_z \sigma_1^z \sigma_2^z + J_{yz} \sigma_1^y \sigma_2^z + J_{zy} \sigma_1^z \sigma_2^y. \quad (18)$$

The latter can be rewritten in the form

$$\begin{aligned} \mathcal{H}_{xx} = & B_1^x \sigma_1^x + B_2^x \sigma_2^x + J_x \sigma_1^x \sigma_2^x + J_y \sigma_1^y \sigma_2^y + J_z \sigma_1^z \sigma_2^z \\ & + D_x (\sigma_1^y \sigma_2^z - \sigma_1^z \sigma_2^y) + \Gamma_x (\sigma_1^y \sigma_2^z + \sigma_1^z \sigma_2^y), \end{aligned} \quad (19)$$

where

$$D_x = \frac{1}{2}(J_{yz} - J_{zy}), \quad \Gamma_x = \frac{1}{2}(J_{yz} + J_{zy}) \quad (20)$$

are the x -components of Dzyaloshinsky vector and $\tilde{\Gamma}$ tensor, respectively.

So here we have the two-qubit anisotropic Heisenberg spin cluster with D_x and Γ_x terms of DM and KSEA interactions and additionally in the nonuniform external fields applied in the transverse x -direction.

In Ref. [47] and then in Refs. [36,37], it has been shown that by means of double Hadamard transformation $H \otimes H$, where

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = H^t \tag{21}$$

is the Hadamard transform, any CS matrix 4×4 is reduced to the X form (and vice versa). Indeed, taking into account relations

$$H\sigma_x H = \sigma_z, \quad H\sigma_y H = -\sigma_y, \quad H\sigma_z H = \sigma_x \tag{22}$$

simple calculations yield

$$\begin{aligned} (H \otimes H)\mathcal{H}_{xx}(H \otimes H) &= B_1^x \sigma_1^z + B_2^x \sigma_2^z + J_z \sigma_1^x \sigma_2^x + J_y \sigma_1^y \sigma_2^y + J_x \sigma_1^z \sigma_2^z \\ &+ D_x (\sigma_1^x \sigma_2^y - \sigma_1^y \sigma_2^x) - \Gamma_x (\sigma_1^x \sigma_2^y + \sigma_1^y \sigma_2^x). \end{aligned} \tag{23}$$

Thus, the CS Hamiltonian is returned to the X case up to a reassignment of seven parameters.

As a result, the discovered remarkable transformation $H \otimes H$ allows to find correlation functions using the corresponding solutions for the X states. Knowing the solution for X state, we now able to calculate such quantum correlations as quantum entanglement, discord, and one-way work deficit for the CS case of XYZ model in the transverse external fields and not only with DM but also with KSEA interaction.

5 Group-theoretical view on the quantum states

To find the key to solve the XYZ model with the components D_y and Γ_y of the DM and KSEA interactions, we analyze the symmetry of the CS matrix using group-theoretical methods. In addition, in the future this case will serve us as a heuristic example.

In the most general case, the four-by-four CS matrix is written as

$$A_{CS} = \begin{pmatrix} A_1 & A_2 & A_3 & A_4 \\ A_5 & A_6 & A_7 & A_8 \\ A_8 & A_7 & A_6 & A_5 \\ A_4 & A_3 & A_2 & A_1 \end{pmatrix}, \tag{24}$$

where the entries are arbitrary real or complex values. The CS matrix is symmetric about its center. On the other hand, we may say that CS matrix is such a matrix that commutes with the operator [48]

$$U_{xx} = \begin{pmatrix} \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot \end{pmatrix}. \tag{25}$$

Table 1 Character table of the group $\{E, U_{xx}\}$

$\{E, U_{xx}\}$	E	U_{xx}
$\Gamma^{(1)}$	1	1
$\Gamma^{(2)}$	1	-1
Γ	4	0

It is clear that U_{xx}^2 equals the unity matrix. One may also claim that the commutativity condition with this operator generates the CS matrix, i.e., the most general matrix that commutes with U_{xx} is the CS matrix.

Let us find out what consequences the symmetry of matrix (24) lead to. For this purpose, we perform a group-theoretical analysis. The transformation U_{xx} together with the identity transformation E makes up the group $\{E, U_{xx}\}$. This group is of second order and has two irreducible representations $\Gamma^{(1)}$ and $\Gamma^{(2)}$. The 4×4 unit matrix and the matrix (25) together give the original representation Γ of this group in the space of the matrix (24). The characters of Γ (traces of representation matrices) equal $\chi(E) = 4$ and $\chi(U_{xx}) = 0$. Knowing them, we can find the multiplicities a_1 and a_2 with which the irreducible representations $\Gamma^{(1)}$ and $\Gamma^{(2)}$, respectively, are contained in Γ .

For this purpose, it is sufficient to make use of the character table for the group (Table 1) and the formula [49]

$$a_\mu = \frac{1}{g} \sum_G \chi^{(\mu)}(G)^* \chi(G), \tag{26}$$

where g is the order of the group, $\chi^{(\mu)}(G)$ the character of the element G in the μ -th irreducible representation, and $\chi(G)$ the character of the same element in the original representation. Simple calculations yield

$$a_1 = 2, \quad a_2 = 2. \tag{27}$$

This imply that in the basis where the representation Γ of the Abelian group $\{E, U_{xx}\}$ is completely reducible, the matrix (24) will take a block-diagonal form with two subblocks 2×2 .

Quasidiagonalizing transformation is constructed from the eigenvectors of the operator U_{xx} and can be written as

$$R = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \cdot & \cdot & 1 \\ \cdot & 1 & 1 & \cdot \\ \cdot & 1 & -1 & \cdot \\ 1 & \cdot & \cdot & -1 \end{pmatrix} = R^t. \tag{28}$$

This transformation is orthogonal and symmetric (coincides with its transposition). After this transformation, the CS matrix (24) takes the quasidiagonal form

$$R A_{CS} R = \begin{pmatrix} A_1 + A_4 & A_2 + A_3 & \cdot & \cdot \\ A_5 + A_8 & A_6 + A_7 & \cdot & \cdot \\ \cdot & \cdot & A_6 - A_7 & A_5 - A_8 \\ \cdot & \cdot & A_2 - A_3 & A_1 - A_4 \end{pmatrix}. \tag{29}$$

Note that another useful way to practically quasidiagonalize different matrices is to use for them so-called motion integrals [50].

The resulting quasidiagonal form allows it easy to extract all eigenvalues of any CS matrix and, in particular, of the Hamiltonian and density matrix. In turn, in some cases, this opens a possibility to direct calculation of quantum correlations, for example the quantum entanglement of two-qubit quantum CS states [51].

Importantly, the matrix U_{xx} can be written as a direct product of Pauli matrices,

$$U_{xx} = \sigma_x \otimes \sigma_x. \tag{30}$$

It is this property that allowed to reduce the problem to the known case by applying the local unitary transformation (double Hadamard transformation) and calculate any quantum correlations of CS states using the results for the X quantum states.

It is arisen a question either to consider another combinations $U_{\alpha\beta} = \sigma_\alpha \otimes \sigma_\beta$ ($\alpha, \beta = 0, x, y, z$) with all possible Pauli matrices including the unit matrix σ_0 . Take, for instance,

$$U_{zz} = \sigma_z \otimes \sigma_z = \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & -1 & \cdot & \cdot \\ \cdot & \cdot & -1 & \cdot \\ \cdot & \cdot & \cdot & 1 \end{pmatrix}. \tag{31}$$

Simple calculations show that the most general matrix that commutes with U_{zz} has the X form:

$$A_X = \begin{pmatrix} A_1 & \cdot & \cdot & A_2 \\ \cdot & A_3 & A_4 & \cdot \\ \cdot & A_5 & A_6 & \cdot \\ A_7 & \cdot & \cdot & A_8 \end{pmatrix}. \tag{32}$$

So we can now give a new definition for the X matrix; namely, it is such a matrix that commutes with the matrix $U_{zz} = \sigma_z \otimes \sigma_z$ or, in other words, is invariant under the transformations of the group $\{E, U_{zz}\}$.

In the following sections, we will continue to develop such a group-theoretical approach.

6 XYZ chain with D_y and Γ_y couplings

We return to the consideration of spin systems. Let us now take the direct product of two σ_y matrices,

$$U_{yy} = \sigma_y \otimes \sigma_y = \begin{pmatrix} \cdot & \cdot & \cdot & -1 \\ \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot \\ -1 & \cdot & \cdot & \cdot \end{pmatrix}, \tag{33}$$

and find the most general matrix that commutes with it. Carrying out the necessary calculations, we get the matrix

$$A_{yy} = \begin{pmatrix} A_1 & A_2 & A_3 & A_4 \\ A_5 & A_6 & A_7 & A_8 \\ -A_8 & A_7 & A_6 & -A_5 \\ A_4 & -A_3 & -A_2 & A_1 \end{pmatrix}. \tag{34}$$

Note that a family of matrices with such a structure is algebraically closed.

Again performing a group-theoretical analysis, as in previous section, we find that the matrix (34) can be reduced to a block-diagonal form also with two subblocks of second orders. The quasidiagonalizing transformation is built from eigenvectors of U_{yy} , Eq. (33), and can be written as

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & \cdot & \cdot & 1 \\ \cdot & 1 & 1 & \cdot \\ \cdot & 1 & -1 & \cdot \\ 1 & \cdot & \cdot & 1 \end{pmatrix} = S^t. \tag{35}$$

Calculations yield

$$SA_{yy}S = \begin{pmatrix} A_1 - A_4 & -A_2 - A_3 & \cdot & \cdot \\ -A_5 + A_8 & A_6 + A_7 & \cdot & \cdot \\ \cdot & \cdot & A_6 - A_7 & A_5 + A_8 \\ \cdot & \cdot & A_2 - A_3 & A_1 + A_4 \end{pmatrix}. \tag{36}$$

This results opens a way to extract all eigenvalues of any A_{yy} matrix.

Taking into account hermiticity condition, one can write the density matrix with the discussed symmetry:

$$\rho_{yy} = \begin{pmatrix} a & \mu & v & c \\ \mu^* & b & d & -v^* \\ v^* & d & b & -\mu^* \\ c & -v & -\mu & a \end{pmatrix}. \tag{37}$$

Similar structure has the Hamiltonian

$$\mathcal{H}_{yy} = \begin{pmatrix} J_z & -iB_2^y + J_{zx} & -iB_1^y + J_{xz} & J_x - J_y \\ iB_2^y + J_{zx} & -J_z & J_x + J_y & -iB_1^y - J_{xz} \\ iB_1^y + J_{xz} & J_x + J_y & -J_z & -iB_2^y - J_{zx} \\ J_x - J_y & iB_1^y - J_{xz} & iB_2^y - J_{zx} & J_z \end{pmatrix}. \tag{38}$$

In the Bloch form, this Hamiltonian is given by

$$\mathcal{H}_{yy} = B_1^y \sigma_1^y + B_2^y \sigma_2^y + J_x \sigma_1^x \sigma_2^x + J_y \sigma_1^y \sigma_2^y + J_z \sigma_1^z \sigma_2^z + J_{zx} \sigma_1^z \sigma_2^x + J_{xz} \sigma_1^x \sigma_2^z. \tag{39}$$

In terms of the DM and KSEA couplings, this equation is rewritten as

$$\begin{aligned} \mathcal{H}_{yy} = & B_1^y \sigma_1^y + B_2^y \sigma_2^y + J_x \sigma_1^x \sigma_2^x + J_y \sigma_1^y \sigma_2^y + J_z \sigma_1^z \sigma_2^z \\ & + D_y (\sigma_1^z \sigma_2^x - \sigma_1^x \sigma_2^z) + \Gamma_y (\sigma_1^z \sigma_2^x + \sigma_1^x \sigma_2^z), \end{aligned} \tag{40}$$

where

$$D_y = \frac{1}{2}(J_{zx} - J_{xz}), \quad \Gamma_y = \frac{1}{2}(J_{zx} + J_{xz}) \tag{41}$$

are the y-components of Dzyaloshinsky vector and $\vec{\Gamma}$ tensor, respectively. So, we come to the completely anisotropic Heisenberg modes in the “transverse” external field and with independent D_y and Γ_y terms of DM and KSEA interactions.

As already noted above, it is important to find *local* unitary transformations. The Hadamard transform diagonalizes the spin matrix σ_x . It easy to check that the Pauli matrix σ_y is diagonalized by the unitary transformation

$$Y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}. \tag{42}$$

(This operator can be called a *Y*-transform because it diagonalizes the matrix σ_y .) In the proper representation of the matrix σ_y ,¹

$$Y^\dagger \sigma_x Y = \sigma_y, \quad Y^\dagger \sigma_y Y = \sigma_z, \quad Y^\dagger \sigma_z Y = \sigma_x. \tag{43}$$

Double transformation of *Y* reduces the Hamiltonian \mathcal{H}_{yy} to the X form. Indeed,

$$\begin{aligned} (Y \otimes Y)^\dagger \mathcal{H}_{yy} (Y \otimes Y) = & B_1^y \sigma_1^z + B_2^y \sigma_2^z + J_z \sigma_1^x \sigma_2^x + J_x \sigma_1^y \sigma_2^y + J_y \sigma_1^z \sigma_2^z \\ & + D_y (\sigma_1^x \sigma_2^y - \sigma_1^y \sigma_2^x) + \Gamma_y (\sigma_1^x \sigma_2^y + \sigma_1^y \sigma_2^x). \end{aligned} \tag{44}$$

The same is valid for the density matrix ρ_{yy} : It is also reduced to the X form by the local unitary transformation consisting of direct product of two *Y* transforms.

¹ One may also choose $\tilde{Y} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$ that leads to the relations $\tilde{Y}^\dagger \sigma_x \tilde{Y} = \sigma_x$, $\tilde{Y}^\dagger \sigma_y \tilde{Y} = \sigma_z$, and $\tilde{Y}^\dagger \sigma_z \tilde{Y} = -\sigma_y$.

So, we have found a way which allows to calculate the quantum correlations in the XYZ system with arbitrary components D_y and Γ_y using the known formulas for the X states. At the same time, the way found shows the equivalence of quantum correlation properties in the system under discussion and in the X (and CS) system.

7 Classification of quantum states

The examples considered in the previous sections provide us with a starting point to explore the invariance under local operations to extend the known results and get new quantum states. Consider now the mixed products of spin matrices²

$$U_{\alpha\beta} = \sigma_\alpha \otimes \sigma_\beta \quad (\alpha, \beta = 0, x, y, z), \quad (45)$$

where $\sigma_0, \sigma_x, \sigma_y,$ and σ_z are given by Eq. (12). The matrices commuting with each given operator $U_{\alpha\beta}$ form algebraically closed families. One should be noted that such U -operators, up to common coefficients, coincide with the generators of SU(4) group [52–55].

Repeating calculations similar to Sect. 5, we find, as above, that the characters of the initial representation of any group $\{E, U_{\alpha\beta}\}$ are still equal to four and zero, and therefore, the multiplicities are again $a_1 = a_2 = 2$. As a result, any matrix that commutes with the matrix $U_{\alpha\beta}$ can be reduced to the block-diagonal form with two subblocks of second order. Quasidiagonalizing transformations are constructed from the eigenvectors of the given matrix $U_{\alpha\beta}$.

Finding for each operator $U_{\alpha\beta}$ the matrix originated from the condition of commutativity and then taking its Hermitian form, we arrive at a collection of quantum states (and Hamiltonians) which is shown in Table 2.

Each quantum state (and hence Hamiltonian) is supplied by a set of Pauli matrices over which the quantum state or Hamiltonian is decomposed in the form of a linear combination.

We can look at Table 2 as a four-by-four matrix. Using this table, it is easy to find the Hamiltonians and density matrices of different spin models. Let us consider the first row. The corresponding Hamiltonians are written as

$$\mathcal{H}_{0x} = \mathbf{B}_1 \sigma_1 + B_2^x \sigma_2^x + J_x \sigma_1^x \sigma_2^x + J_{zx} \sigma_1^z \sigma_2^x + J_{yx} \sigma_1^y \sigma_2^x, \quad (46)$$

$$\mathcal{H}_{0y} = \mathbf{B}_1 \sigma_1 + B_2^y \sigma_2^y + J_y \sigma_1^y \sigma_2^y + J_{zy} \sigma_1^z \sigma_2^y + J_{xy} \sigma_1^x \sigma_2^y, \quad (47)$$

$$\mathcal{H}_{0z} = \mathbf{B}_1 \sigma_1 + B_2^z \sigma_2^z + J_z \sigma_1^z \sigma_2^z + J_{yz} \sigma_1^y \sigma_2^z + J_{xz} \sigma_1^x \sigma_2^z. \quad (48)$$

System (46) by means of local unitary transform $\sigma_0 \otimes H$ and system (47) by the local unitary transformation $\sigma_0 \otimes Y$ are reduced to a structure of the model (48):

$$(\sigma_0 \otimes H) \mathcal{H}_{0x} (\sigma_0 \otimes H) \rightarrow \mathcal{H}_{0z}, \quad (\sigma_0 \otimes Y) \dagger \mathcal{H}_{0y} (\sigma_0 \otimes Y) \rightarrow \mathcal{H}_{0z}. \quad (49)$$

Thus, all quantum correlations in these three spin systems are the same.

² We omit the case $U_{00}(= E)$ because $\{E\}$ is the trivial group.

Table 2 Fifteen quantum states/Hamiltonians generated by U -operators and, in braces, spin matrix septets required for their Bloch decompositions

$U_{x0} = \sigma_x \otimes \sigma_0$ $\mathcal{H}_{0x}, \rho_{0x}$: $\begin{pmatrix} a & c & v & \gamma \\ c & a & \gamma & v \\ v^* & \gamma^* & b & d \\ \gamma^* & v^* & d & b \end{pmatrix}$ $\{\sigma_1^x, \sigma_1^y, \sigma_1^z, \sigma_2^x, \sigma_2^y, \sigma_2^z, \sigma_1^x \sigma_2^x, \sigma_1^y \sigma_2^y, \sigma_1^z \sigma_2^z, \sigma_1^x \sigma_2^y, \sigma_1^y \sigma_2^x, \sigma_1^z \sigma_2^x, \sigma_1^x \sigma_2^z, \sigma_1^y \sigma_2^z, \sigma_1^z \sigma_2^y\}$ $U_{xx} = \sigma_x \otimes \sigma_x$ $\mathcal{H}_{xx}, \rho_{xx}$: $\begin{pmatrix} a & \mu & v & c \\ \mu^* & b & d & v^* \\ v^* & d & b & \mu^* \\ c & v & \mu & a \end{pmatrix}$ $\{\sigma_1^x, \sigma_2^x, \sigma_1^y, \sigma_2^y, \sigma_1^z, \sigma_2^z, \sigma_1^x \sigma_2^x, \sigma_1^y \sigma_2^y, \sigma_1^z \sigma_2^z, \sigma_1^x \sigma_2^y, \sigma_1^y \sigma_2^x, \sigma_1^z \sigma_2^x, \sigma_1^x \sigma_2^z, \sigma_1^y \sigma_2^z, \sigma_1^z \sigma_2^y\}$	$U_{0y} = \sigma_0 \otimes \sigma_y$ $\mathcal{H}_{0y}, \rho_{0y}$: $\begin{pmatrix} a & i\mu & v & \gamma \\ -i\mu & a & -\gamma & v \\ v^* & -\gamma^* & b & i\delta \\ \gamma^* & v^* & -i\delta & b \end{pmatrix}$ $\{\sigma_1^x, \sigma_1^y, \sigma_1^z, \sigma_2^x, \sigma_2^y, \sigma_1^x \sigma_2^y, \sigma_1^y \sigma_2^x, \sigma_1^z \sigma_2^z, \sigma_1^x \sigma_2^z, \sigma_1^y \sigma_2^z, \sigma_1^z \sigma_2^y\}$ $U_{xy} = \sigma_x \otimes \sigma_y$ $\mathcal{H}_{xy}, \rho_{xy}$: $\begin{pmatrix} a & \mu & v & i\gamma \\ \mu^* & b & i\delta & v^* \\ v^* & -i\delta & b & -\mu^* \\ -i\gamma & v & -\mu & a \end{pmatrix}$ $\{\sigma_1^x, \sigma_2^y, \sigma_1^z \sigma_2^z, \sigma_1^x \sigma_2^x, \sigma_1^y \sigma_2^y, \sigma_1^x \sigma_2^y, \sigma_1^y \sigma_2^x, \sigma_1^z \sigma_2^x, \sigma_1^x \sigma_2^z, \sigma_1^y \sigma_2^z, \sigma_1^z \sigma_2^y\}$	$U_{0z} = \sigma_0 \otimes \sigma_z$ $\mathcal{H}_{0z}, \rho_{0z}$: $\begin{pmatrix} a & . & v & . \\ . & b & . & \delta \\ v^* & . & c & . \\ . & \delta^* & . & d \end{pmatrix}$ $\{\sigma_1^x, \sigma_1^y, \sigma_1^z, \sigma_2^x, \sigma_2^y, \sigma_1^x \sigma_2^z, \sigma_1^y \sigma_2^z, \sigma_1^z \sigma_2^y, \sigma_1^x \sigma_2^y, \sigma_1^y \sigma_2^x, \sigma_1^z \sigma_2^x, \sigma_1^x \sigma_2^z, \sigma_1^y \sigma_2^z, \sigma_1^z \sigma_2^y\}$ $U_{xz} = \sigma_x \otimes \sigma_z$ $\mathcal{H}_{xz}, \rho_{xz}$: $\begin{pmatrix} a & \mu & c & \gamma \\ \mu^* & b & -\gamma^* & d \\ c & -\gamma & a & -\mu \\ \gamma^* & d & -\mu^* & b \end{pmatrix}$ $\{\sigma_1^x, \sigma_2^z, \sigma_1^y \sigma_2^z, \sigma_1^x \sigma_2^x, \sigma_1^y \sigma_2^y, \sigma_1^z \sigma_2^z, \sigma_1^x \sigma_2^y, \sigma_1^y \sigma_2^x, \sigma_1^z \sigma_2^x, \sigma_1^x \sigma_2^z, \sigma_1^y \sigma_2^z, \sigma_1^z \sigma_2^y\}$
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Table 2 continued

$U_{y0} = \sigma_y \otimes \sigma_0$ $\mathcal{H}_{y0}, \rho_{y0}$: $\begin{pmatrix} a & \mu & \nu & \gamma \\ \mu^* & b & -\gamma^* & i\delta \\ -i\nu & \gamma & a & \mu \\ \gamma^* & -i\delta & \mu^* & b \end{pmatrix}$ $\{\sigma_1^y, \sigma_2^y, \sigma_2^z, \sigma_2^x\}$ $\sigma_1^y \sigma_2^y$ $\sigma_1^y \sigma_2^z$ $\sigma_1^y \sigma_2^x$	$U_{yx} = \sigma_y \otimes \sigma_x$ $\mathcal{H}_{yx}, \rho_{yx}$: $\begin{pmatrix} a & \mu & \nu & i\gamma \\ \mu^* & b & i\delta & -\nu^* \\ \nu^* & -i\delta & b & \mu^* \\ -i\gamma & -\nu & \mu & a \end{pmatrix}$ $\{\sigma_1^y, \sigma_2^y, \sigma_1^z, \sigma_2^z, \sigma_1^x, \sigma_2^x, \sigma_1^y \sigma_2^x, \sigma_1^z \sigma_2^x, \sigma_1^y \sigma_2^z, \sigma_1^z \sigma_2^y\}$ $U_{zx} = \sigma_z \otimes \sigma_x$ $\mathcal{H}_{zx}, \rho_{zx}$: $\begin{pmatrix} a & c & \nu & \gamma \\ c & a & -\gamma & -\nu \\ \nu^* & -\gamma^* & b & d \\ \gamma^* & -\nu^* & d & b \end{pmatrix}$ $\{\sigma_1^z, \sigma_2^z, \sigma_1^y \sigma_2^z, \sigma_1^x \sigma_2^z, \sigma_1^y \sigma_2^x, \sigma_1^x \sigma_2^y, \sigma_1^y \sigma_2^x \sigma_2^z, \sigma_1^x \sigma_2^y \sigma_2^z\}$	$U_{yy} = \sigma_y \otimes \sigma_y$ $\mathcal{H}_{yy}, \rho_{yy}$: $\begin{pmatrix} a & \mu & \nu & c \\ \mu^* & b & d & -\nu^* \\ \nu^* & d & b & -\mu^* \\ c & -\nu & -\mu & a \end{pmatrix}$ $\{\sigma_1^y, \sigma_2^y, \sigma_1^x \sigma_2^x, \sigma_1^y \sigma_2^y, \sigma_1^z \sigma_2^z, \sigma_1^y \sigma_2^z, \sigma_1^z \sigma_2^y, \sigma_1^x \sigma_2^z, \sigma_1^y \sigma_2^x\}$ $U_{zy} = \sigma_z \otimes \sigma_y$ $\mathcal{H}_{zy}, \rho_{zy}$: $\begin{pmatrix} a & i\mu & \nu & \gamma \\ -i\mu & a & \gamma & -\nu \\ \nu^* & \gamma^* & b & i\delta \\ \gamma^* & -\nu^* & -i\delta & b \end{pmatrix}$ $\{\sigma_1^z, \sigma_2^z, \sigma_1^x \sigma_2^x, \sigma_1^y \sigma_2^y, \sigma_1^z \sigma_2^z, \sigma_1^y \sigma_2^z, \sigma_1^z \sigma_2^y, \sigma_1^x \sigma_2^z, \sigma_1^y \sigma_2^x\}$	$U_{yz} = \sigma_y \otimes \sigma_z$ $\mathcal{H}_{yz}, \rho_{yz}$: $\begin{pmatrix} a & \mu & \nu & \gamma \\ \mu^* & b & \gamma^* & i\delta \\ -i\nu & \gamma & a & -\mu \\ \gamma^* & -i\delta & -\mu^* & b \end{pmatrix}$ $\{\sigma_1^y, \sigma_2^z, \sigma_1^x \sigma_2^x, \sigma_1^y \sigma_2^z, \sigma_1^z \sigma_2^z, \sigma_1^y \sigma_2^x, \sigma_1^z \sigma_2^y, \sigma_1^x \sigma_2^z, \sigma_1^y \sigma_2^x\}$ $U_{zz} = \sigma_z \otimes \sigma_z$ $\mathcal{H}_{zz}, \rho_{zz}$: $\begin{pmatrix} a & \cdot & \gamma \\ \cdot & b & \delta \\ \cdot & \delta^* & c \\ \gamma^* & \cdot & d \end{pmatrix}$ $\{\sigma_1^z, \sigma_2^z, \sigma_1^x \sigma_2^x, \sigma_1^y \sigma_2^y, \sigma_1^z \sigma_2^z, \sigma_1^y \sigma_2^z, \sigma_1^z \sigma_2^y, \sigma_1^x \sigma_2^z, \sigma_1^y \sigma_2^x\}$
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The mixed members can be rewritten through the DM and KSEA interactions. For example,

$$\begin{aligned} \mathcal{H}_{0z} = & \mathbf{B}_1\sigma_1 + B_2^z\sigma_2^z + J_z\sigma_1^z\sigma_2^z + D_x(\sigma_1^y\sigma_2^z - \sigma_1^z\sigma_2^y) + \Gamma_x(\sigma_1^y\sigma_2^z + \sigma_1^z\sigma_2^y) \\ & + D_y(\sigma_1^z\sigma_2^x - \sigma_1^x\sigma_2^z) + \Gamma_y(\sigma_1^z\sigma_2^x + \sigma_1^x\sigma_2^z) \end{aligned} \tag{50}$$

with additional conditions $\Gamma_x = D_x$ and $\Gamma_y = -D_y$ in accord with Eqs. (20) and (41). The corresponding density matrix has a characteristic, “checkerboard” structure

$$\rho_{0z} = \begin{pmatrix} a & \cdot & v & \cdot \\ \cdot & b & \cdot & \delta \\ v^* & \cdot & c & \cdot \\ \cdot & \delta^* & \cdot & d \end{pmatrix}. \tag{51}$$

A partial transposition of ρ_{0z} , namely $\rho_{0z}^{t_2}$, does not change the density matrix: $\rho_{0z}^{t_2} = \rho_{0z}$. Consequently, all eigenvalues stay nonnegative, and therefore, in accordance with the positive partial transpose (PPT) criterion [56,57], the state (51) is separable, i.e., its quantum entanglement (and with it the entanglement of systems with the Hamiltonians \mathcal{H}_{0x} and \mathcal{H}_{0y}) is identically equal to zero.

Consider now the systems from the first column of Table 2. They are

$$\mathcal{H}_{x0} = B_1^x\sigma_1^x + \mathbf{B}_2\sigma_2 + J_x\sigma_1^x\sigma_2^x + J_{xy}\sigma_1^x\sigma_2^y + J_{xz}\sigma_1^x\sigma_2^z, \tag{52}$$

$$\mathcal{H}_{y0} = B_1^y\sigma_1^y + \mathbf{B}_2\sigma_2 + J_y\sigma_1^y\sigma_2^y + J_{yx}\sigma_1^y\sigma_2^x + J_{yz}\sigma_1^y\sigma_2^z, \tag{53}$$

$$\mathcal{H}_{z0} = B_1^z\sigma_1^z + \mathbf{B}_2\sigma_2 + J_z\sigma_1^z\sigma_2^z + J_{zx}\sigma_1^z\sigma_2^x + J_{zy}\sigma_1^z\sigma_2^y. \tag{54}$$

The cross (helical) interactions in these Hamiltonians can also be given in the form of DM–KSEA interactions. These models again pass one into another by the local unitary transformations consisting of the corresponding direct products of operators H, Y , and σ_0 . The density matrix corresponding to the Hamiltonian \mathcal{H}_{z0} has a block-diagonal (and therefore direct sum) form (see Table 2)

$$\rho_{z0} = \begin{pmatrix} a & \mu & \cdot & \cdot \\ \mu^* & b & \cdot & \cdot \\ \cdot & \cdot & c & v \\ \cdot & \cdot & v^* & d \end{pmatrix} = \begin{pmatrix} a & \mu \\ \mu^* & b \end{pmatrix} \oplus \begin{pmatrix} c & v \\ v^* & d \end{pmatrix}. \tag{55}$$

The quantum entanglement of this state as well as the states corresponding to the Hamiltonians \mathcal{H}_{x0} and \mathcal{H}_{y0} equals zero, again in accordance with the PPT criterion.

The Hamiltonians (46)–(48) are pairwise connected with the Hamiltonians (52)–(54) using the spin exchange operator P introduced by Dirac (see [32, Sect. 12-2]),

$$P = \frac{1}{2}(1 + \sigma_1\sigma_2) = \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \end{pmatrix} = P^t. \tag{56}$$

This operator exchanges the first and second qubits ($1 \rightleftharpoons 2$) and swaps them (similar to the mirror reflection in the plane that separates the qubits):

$$P\sigma_\alpha \otimes \sigma_\beta P = \sigma_\beta \otimes \sigma_\alpha, \quad P\sigma_1^\alpha \sigma_2^\beta P = \sigma_1^\beta \sigma_2^\alpha. \tag{57}$$

The matrix (56) is an orthogonal transformation that permutes the second and third rows and columns of any matrix of the fourth order. One should emphasize that this transformation is not local, and therefore, generally speaking, it changes the value of quantum correlation because the quantum discord and one-way work deficit depend on which qubit the measurement was performed. As noted in [24,58], the discord is not a symmetric quantity, and there are “left” and “right” discords of the same system. However, if simultaneously with the permutation P , the measured qubit is changed in the discussed systems, then the value of discord (and deficit) will remain unchanged. As an example, $P\rho_{0z}P \rightarrow \rho_{z0}$ and the “right” discord passes to the “left” one and vice versa.

Now we turn to the consideration of the “inner” part of Table 2, i.e., the systems and their quantum states with the Cartesian indexes $\alpha, \beta = x, y, z$ only. “Diagonal” states ($\rho_{xx}, \rho_{yy},$ and ρ_{zz}) have already been discussed in detail in previous sections. All of them are related by local unitary transformations, and therefore, the quantum correlations are the same and can be calculated using formulas available for the X state.

The “off-diagonal” Hamiltonians from the upper triangle part of the table are written as follows

$$\mathcal{H}_{xy} = B_1^x \sigma_1^x + B_2^y \sigma_2^y + J_z \sigma_1^z \sigma_2^z + J_{xy} \sigma_1^x \sigma_2^y + J_{yx} \sigma_1^y \sigma_2^x + J_{yz} \sigma_1^y \sigma_2^z + J_{zx} \sigma_1^z \sigma_2^x, \tag{58}$$

$$\mathcal{H}_{xz} = B_1^x \sigma_1^x + B_2^z \sigma_2^z + J_y \sigma_1^y \sigma_2^y + J_{zx} \sigma_1^z \sigma_2^x + J_{xz} \sigma_1^x \sigma_2^z + J_{zy} \sigma_1^z \sigma_2^y + J_{yx} \sigma_1^y \sigma_2^x, \tag{59}$$

$$\mathcal{H}_{yz} = B_1^y \sigma_1^y + B_2^z \sigma_2^z + J_x \sigma_1^x \sigma_2^x + J_{zy} \sigma_1^z \sigma_2^y + J_{yz} \sigma_1^y \sigma_2^z + J_{zx} \sigma_1^z \sigma_2^x + J_{xy} \sigma_1^x \sigma_2^y. \tag{60}$$

These Hamiltonians can be expressed via DM–KSEA interactions. For instance,

$$\mathcal{H}_{xy} = B_1^x \sigma_1^x + B_2^y \sigma_2^y + J_z \sigma_1^z \sigma_2^z + \mathbf{D} \cdot (\boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2) + \boldsymbol{\sigma}_1 \cdot \tilde{\boldsymbol{\Gamma}} \cdot \boldsymbol{\sigma}_2 \tag{61}$$

with conditions $\Gamma_x = D_x$ and $\Gamma_y = D_y$, whereas Γ_z and D_z are arbitrary independent quantities. The Hamiltonians of a lower part of the “off-diagonal” systems are

$$\mathcal{H}_{yx} = B_1^y \sigma_1^y + B_2^x \sigma_2^x + J_z \sigma_1^z \sigma_2^z + J_{xy} \sigma_1^x \sigma_2^y + J_{yx} \sigma_1^y \sigma_2^x + J_{zy} \sigma_1^z \sigma_2^y + J_{xz} \sigma_1^x \sigma_2^z, \tag{62}$$

$$\mathcal{H}_{zx} = B_1^z \sigma_1^z + B_2^x \sigma_2^x + J_y \sigma_1^y \sigma_2^y + J_{zx} \sigma_1^z \sigma_2^x + J_{xz} \sigma_1^x \sigma_2^z + J_{yz} \sigma_1^y \sigma_2^z + J_{xy} \sigma_1^x \sigma_2^y, \tag{63}$$

$$\mathcal{H}_{zy} = B_1^z \sigma_1^z + B_2^y \sigma_2^y + J_x \sigma_1^x \sigma_2^x + J_{zy} \sigma_1^z \sigma_2^y + J_{yz} \sigma_1^y \sigma_2^z + J_{yx} \sigma_1^y \sigma_2^x + J_{zx} \sigma_1^x \sigma_2^z. \tag{64}$$

Remarkably, all these six “off-diagonal” Hamiltonians (58)–(60) and (62)–(64) are reduced to the Hamiltonian of the X model by local unitary transformations composed of the operators H , Y , and σ_0 . Indeed,

$$(H \otimes Y)^\dagger \mathcal{H}_{xy} (H \otimes Y) \rightarrow \mathcal{H}_{zz}, \quad (H \otimes \sigma_0) \mathcal{H}_{xz} (H \otimes \sigma_0) \rightarrow \mathcal{H}_{zz}, \quad (65)$$

similarly for other cases.

So, out of fifteen quantum states, nine ($\rho_{\alpha\beta}$ with $\alpha, \beta = x, y, z$) are transformed among themselves by local unitary transformations. Their quantum correlations are complete identical to each other and are calculated by the formulas for the X state.

The quantum states of the six remaining models are separable and therefore without quantum entanglement. These models consist of two equal subclasses $\rho_{0\alpha}$ and $\rho_{\alpha 0}$ ($\alpha = x, y, z$) in each of which the quantum discord and other quantum correlations are equivalent to each other since the states are connected via local unitary transformations. Moreover, the states from different subclasses are paired trough the spin exchange transformation P thanks to which the “right” quantum discord of one member of a pair equals the “left” discord of other member of the same pair. Unfortunately, among both subclasses there is no one quantum state for which the quantum discord is known. However, most recently Zhou et al. [59] have evaluated the “right” and “left” quantum discords for the quantum sate

$$\rho = \frac{1}{4}(1 + s_1\sigma_1 + c_3\sigma_1^z\sigma_2^z)$$

(see Theorem 2.3 in their paper [59]). It would be interesting to extend this result to the general “checkerboard” (ρ_{0z}) or two-block- (2×2) -diagonal (ρ_{z0}) quantum states.

8 Results and perspectives

We have analyzed fifteen types of two-spin systems in an external field, with the exchange bounds, and with indirect interactions occurring through the orbital magnetic moments. The structures of Hamiltonians and density matrices are presented in an obvious form (Table 2).

The originality and new feature of our results in comparison with other works [12–20] is that we take into account not only the DM interactions, but also the KSEA ones. The latter interactions make their own changes in the behavior of quantum correlations. For example, in recent work [19] a local minimum was found due to DM couplings (black line in Fig. 6c of Ref. [19]). This behavior is reproduced by the dotted line in Fig. 1. We also performed calculations for nonzero values of the constant Γ_z shown by curves 1 and 2 in Fig. 1. It is seen that the KSEA interactions suppress the local minimum of the quantum discord.

We have classified fifteen types of quantum states, each of which contains seven parameters. A detailed study of the behavior of quantum correlations in them will require a separate extensive work in the future.

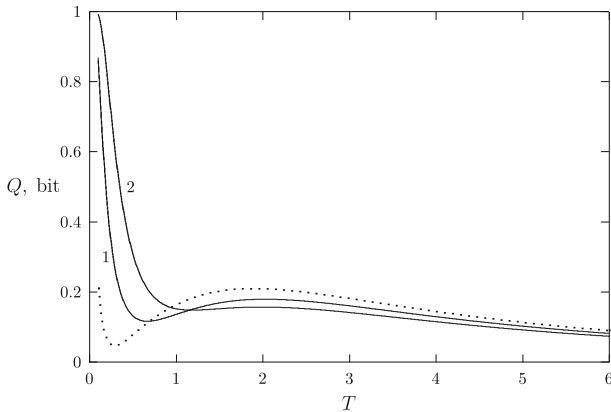


Fig. 1 Quantum discord Q vs temperature T for the model (8) by $B_1^z = B_2^z = 0$, $J_x = -1$, $J_y = -1.5$, $J_z = -2$, $D_z = 1.8$, and $\Gamma_z = 0$ (dotted line), 0.3 (solid line 1), 0.5 (solid line 2)

We have also shown that, from viewpoint of quantum correlation properties, all systems are divided into two groups: the systems with the X quantum states (up to local unitary transformations) for which the developed theory for the calculation of quantum correlations is available and systems with checkerboard-like or block-diagonal non-X quantum states in which the quantum entanglement is absent, whereas the question about the quantum discord and other quantum correlations remains open.

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