Entanglement duality in spin-spin interactions

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We examine entanglement of thermal states for spin-1/2 dimers in external magnetic fields. Entanglement transition in the temperature-magnetic-field plane demonstrates a duality in spin-spin interactions. This identifies a pair of dual categories of symmetric and antisymmetric dimers with each category classified into toric entanglement classes. The entanglement transition line is preserved from each toric entanglement class to its dual toric class. The toric classification is an indication of the topological signature of the entanglement, which bring about topological stability that could be relevant for quantum information processing.

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I. INTRODUCTION

The classification concept has been incorporated in different scientific fields, ranging from biological systems to abstract topology in mathematics in order to categorize relevant objects based on shared characteristics. Scientific classification schemes have not only led to new discoveries of materials and resources, such as in the topological classification of matter [1] and of entangled quantum states [2], but have also helped significantly to find the most efficient and robust approaches to technological advances.

One of the fundamental characteristics of quantum mechanics is the quantum entanglement, which lies at the heart of the difference between the classical and the quantum worlds [3–5]. It is widely believed to be stronger than classical correlations and over the years has become a critically important resource for many applications in quantum technology, including quantum computing, quantum cryptography, quantum communication, and hypersensitive measurements [6]. As a primary attribute of quantum mechanics, quantum entanglement is also much more involved with the foundations, predictions, and interpretations of quantum phenomena. It is strongly linked to the concepts of quantum phase transition and quantum geometric phases [7–12]. Despite significant works having been published, the characteristics of the quantum entanglement is far from a closed topic. New in-depth investigations of existing or entirely new models or systems, continue to enrich this field and to add to the understanding of quantum phenomena, in general.

Here we use entanglement in terms of concurrence [13,14] from a classification perspective in order to analyze spin-spin interactions in atomic dimers and to classify them into entanglement classes. To this end, we focus on the entanglement transition line for thermal states of a generic traceless spin-pair model in the external parameter space specified by temperature (T) and applied magnetic-field (B). We classify the system into a pair of dual categories of symmetric and antisymmetric dimers. Each category consists of toric entanglement classes where each class and its dual are distinguished by the same entanglement transition line on the T-B plane. As a nontrivial example, we introduce dual symmetric and antisymmetric Heisenberg spin-pair interactions and specify their toric entanglement classes. We note that in Ref. [15], the entanglement between two spins in a one-dimensional Heisenberg chain has been studied as a function of temperature and external magnetic field, but not from the classification approach, which is the main focus here. We also note here that the chosen system, the dimer, is not only an excellent model system, it also has real physical relevance since atomic clusters of any size or shape can be realized experimentally, e.g., as ad-atoms on a substrate [16].

II. GENERAL MODEL HAMILTONIAN

We start with a generic traceless spin-pair model described by the Hamiltonian (note that we use $\hbar = 1$ throughout the
paper),
\[ H(\omega, J) = \frac{B_+}{2} s_z^{(1)} + \frac{B_-}{2} s_z^{(2)} + s_i \cdot J s_j, \tag{1} \]
with \( s^{(n)} = (s_x^{(n)}, s_y^{(n)}, s_z^{(n)}) \) being the spin vector operator acting on spins at site \( n = 1, 2 \) of the dimer. We also have that
\[ \mathbf{J} = \begin{pmatrix} J_{xx} & J_{xy} & 0 \\ J_{yx} & J_{yy} & 0 \\ 0 & 0 & J_{zz} \end{pmatrix}, \tag{2} \]
which is a real-valued matrix describing the essential exchange interactions between the two spins. The matrix elements of this matrix are as follows:
\[ J_{xx} = J + r, \quad J_{yy} = J - r, \]
\[ J_{xy} = K - D, \quad J_{yx} = K + D, \]
\[ B_\pm = \omega \pm \Delta. \]

This model accounts for a wide range of important spin-spin interaction systems, including the Heisenberg interaction \( (J_x = J) \), the Dzyaloshinskii-Moriya \( (D) \) interaction, the symmetric anisotropic exchange \( (K) \), as well as anisotropy of the exchange on the XY plane \( (r) \). It further allows for the spins to interact differently with the external magnetic-field \( (B_\pm) \), due to field inhomogeneities. From a physical point of view this would best be performed by studies of magnetic dimers as ad-atoms on an overlay with heterogeneous magnetic structure, or by investigations of dimers with different magnetization direction for the two sites.

The two-qubit Hamiltonian [corresponding to \( s_z = \pm 1/2 \) in Eq. (1)] is chosen so as to ensure that the thermal equilibrium state at temperature \( T \) is of the X type, i.e.,
\[ \mathcal{Q}_T = \frac{1}{2} e^{-H/T} = \begin{pmatrix} \rho_{11} & 0 & 0 & \rho_{14} \\ 0 & \rho_{22} & \rho_{23} & 0 \\ 0 & \rho_{32} & \rho_{33} & 0 \\ \rho_{41} & 0 & 0 & \rho_{44} \end{pmatrix}, \tag{4} \]
in the ordered product qubit-qubit basis \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\} and Boltzmann’s constant is absorbed in \( T \). Explicitly, we have
\[ \rho_{11} = \frac{1}{2} e^{-(J_x/4T)} \left[ \cos \frac{\epsilon_1}{2T} - \sinh \frac{\epsilon_1}{2T} \cos \vartheta \right], \]
\[ \rho_{44} = \frac{1}{2} e^{-(J_x/4T)} \left[ \cosh \frac{\epsilon_1}{2T} + \sinh \frac{\epsilon_1}{2T} \cos \vartheta \right], \]
\[ \rho_{14} = \rho_{41} = -\frac{1}{2} e^{-(J_x/4T)} e^{-i\varphi} \sinh \frac{\epsilon_1}{2T} \sin \vartheta, \tag{5} \]
\[ \rho_{22} = \frac{1}{2} e^{i\varphi/4T} \left[ \cosh \frac{\epsilon_2}{2T} - \sinh \frac{\epsilon_2}{2T} \cos \vartheta \right], \]
\[ \rho_{33} = \frac{1}{2} e^{i\varphi/4T} \left[ \cosh \frac{\epsilon_2}{2T} + \sinh \frac{\epsilon_2}{2T} \cos \vartheta \right], \]
\[ \rho_{23} = \rho_{32} = -\frac{1}{2} e^{i\varphi/4T} e^{-i\varphi} \sin \frac{\epsilon_2}{2T} \sin \vartheta, \]
where
\[ \tan \theta = \frac{\sqrt{r^2 + K^2}}{\omega}, \quad \tan \varphi = \frac{K}{r}, \]
\[ \epsilon_1 = \sqrt{\omega^2 + r^2 + K^2}, \quad \epsilon_2 = \sqrt{\Delta^2 + J^2 + D^2}, \quad \text{and} \quad Z = 2(e^{-J_x/4T}) \cosh \frac{\epsilon_1}{2T} + e^{i\varphi/4T} \cosh \frac{\epsilon_2}{2T} \]
the partition function.

The above X-state form is suitable in our analysis for two reasons: (i) as pointed out before, it accounts for thermal states of several important spin-spin interaction models, and (ii) the entanglement measure concurrence \( C(\mathcal{Q}_T) \) can be calculated analytically. Indeed, one finds [17]
\[ C(\mathcal{Q}_T) = 2 \max(C_1, C_2), \tag{7} \]
where
\[ C_1 = |\rho_{14}| - \sqrt{\rho_{22}\rho_{33}}, \quad C_2 = |\rho_{23}| - \sqrt{\rho_{11}\rho_{44}}. \tag{8} \]

We continue the analysis by exploring the entanglement transition for which one may solve
\[ \max(C_1, C_2) = 0, \tag{9} \]
to extract the critical line in the temperature-magnetic-field parameter space. Equation (9) gives rise to the following duality:
\[ \begin{align*}
(\text{I}) & \quad C_2 \leq C_1 = 0, \\
(\text{II}) & \quad C_1 \leq C_2 = 0,
\end{align*} \tag{10} \]
which becomes
\[ \begin{align*}
(\text{I}) & \quad e^{-(J_x/4T)} p^2 - e^{i\varphi/4T} q^2 = e^{2J_x/4T}, \\
(\text{II}) & \quad e^{i\varphi/4T} q^2 - e^{-(J_x/4T)} p^2 = e^{-(2J_x/4T)} \tag{11}
\end{align*} \]
for our model system with \( p = f(\epsilon_1, \nu) \) and \( q = f(\epsilon_2, \theta) \) given by the function \( f(x, y) = \sin \frac{x}{4T} \sin y \).

This duality relation allows us to categorize the spin-spin interactions in dimers into a pair of dual categories of interactions. We continue by focusing on symmetric and antisymmetric dimers in the sense that the two spins of same magnitude forming the dimer are either parallel and antiparallel. For each case the corresponding Hamiltonian has the following form:

(1) **Symmetric case.** For parallel magnetic moments we would in the simplest case have \( \Delta = 0 \) and \( B_+ = B_- = \omega \). Therefore, interactions of symmetric dimers can be described by the following Hamiltonian:
\[ H_s = \frac{B_+}{2} \left[ s_z^{(1)} + s_z^{(2)} \right] + J_{xz} s_x^{(1)} s_x^{(2)} \]
\[ + J_{yz} s_y^{(1)} s_y^{(2)} - D \left[ s_x^{(1)} s_y^{(2)} - s_y^{(1)} s_x^{(2)} \right] \]
\[ + r \left[ s_x^{(1)} s_z^{(2)} - s_z^{(1)} s_x^{(2)} \right] + K \left[ s_y^{(1)} s_y^{(2)} + s_y^{(1)} s_y^{(2)} \right]. \tag{12} \]

Note that \( \Delta = 0 \) implies \( \theta = \pi/2 \).

(2) **Antisymmetric case.** In the case of antiparallel magnetic moments, we would in the simplest form have \( \omega = 0 \) and \( B_+ = -B_- = \Delta \), the interactions of antisymmetric dimers
\[ H_a = \frac{B_+}{2} \left[ s_z^{(1)} + s_z^{(2)} \right] + \mathbf{J}_{xx} s_x^{(1)} s_x^{(2)} \]
\[ + \mathbf{J}_{yy} s_y^{(1)} s_y^{(2)} - D \left[ s_x^{(1)} s_y^{(2)} - s_y^{(1)} s_x^{(2)} \right] \]
\[ + r \left[ s_x^{(1)} s_z^{(2)} - s_z^{(1)} s_x^{(2)} \right] + K \left[ s_y^{(1)} s_y^{(2)} + s_y^{(1)} s_y^{(2)} \right]. \]
can be described by
\begin{equation}
H_\nu = \frac{B}{2} \left[ s^{(1)}_x s^{(2)}_z - J D s^{(1)}_y s^{(2)}_y \right]
+ r \left[ s^{(1)}_x s^{(2)}_z s^{(1)}_y s^{(2)}_y - D \left( s^{(1)}_s s^{(2)}_s + s^{(1)}_s s^{(2)}_s \right) \right]
+ \tilde{K} \left[ s^{(1)}_s s^{(2)} + s^{(1)}_s s^{(2)}_s \right].
\end{equation}

These relations compared to the ones given in Eq. (15) indicate that the dual symmetric and antisymmetric entanglement classes have the same toric characteristic but with their longitudinal or meridian circles in swapped order as depicted in Fig. 2.

Although the above analysis focuses on concurrence, it is generally independent of the quantum entanglement measure as it is mainly based on the entanglement transition line on the T-B plane. For instance, one can obtain exactly the same classification and entanglement duality using nonlocality [18,19] and negativity [20]. Note that similar to nonlocality, negativity does not, in general, share the same features with concurrence [21,22]. Other than the entanglement duality, our analysis establishes the topological signature of quantum entanglement in a sense that the entanglement phase diagram in dimers provides a clear topological foliation of the coupling parameters manifold into two-dimensional compact torus leaves [23]. Moreover, the toric classifications given in Eqs. (15) and (16) verify that any sets of coupling parameters on the equivalent dual tori give rise to the same entanglement transition line and indeed the same entanglement region on the T-B plane. In other words, as long as the coupling parameters change within the dual tori specified by Eqs. (15) and (16) the entanglement characteristics of the thermal state remain invariant on the T-B plane. This implies a topological stability, namely, robustness of the entanglement in spin-1/2 dimers against variations of the coupling parameters in larger topological domain.

To further clarify our point and show that the entanglement analysis above provides a nontrivial classification and duality, we consider two examples in the following section.

III. EXAMPLES

Consider two identical spin-1/2 particles with Heisenberg spin-spin exchange interaction of strength J in an external magnetic field as given by the Hamiltonian,
\begin{equation}
H^{\text{HE}} = \frac{B}{2} \left[ s^{(1)}_z + s^{(2)}_z \right] + J s^{(1)} \cdot s^{(2)}.
\end{equation}

Note that we use superscript HE here to indicate a Hamiltonian of pure Heisenberg form. In the analysis that follows, we
consider antiferromagnetic coupling $J > 0$ as entanglement cannot occur for ferromagnetic coupling [15]. According to the above classification, the Heisenberg model belongs to a class of symmetric dimers described by the following general form of the Hamiltonian,

$$H_{s}^{\text{HE}} = \frac{B}{2} \left[ s_{x}^{(1)}(1) + s_{z}^{(2)}(1) \right] + J s_{c}^{(1)}(1) s_{c}^{(2)} + J s_{c}^{(1)} s_{z}^{(2)} + D' \left[ s_{x}^{(1)} s_{x}^{(2)} - s_{y}^{(1)} s_{y}^{(2)} \right],$$

such that

$$J'^{2} + D'^{2} = J^{2}. \tag{18}$$

Note that $H_{s}^{\text{HE}} = H_{s}^{\text{HE}}$ for $D' = 0$ and $J' = J$. This accompanies the dual-antisymmetric Heisenberg model described by the Hamiltonian,

$$H_{s}^{\text{AS}} = \frac{B}{2} \left[ s_{x}^{(1)}(1) - s_{z}^{(2)}(1) \right] - J s_{c}^{(1)} s_{c}^{(2)} + \tilde{\rho} \left[ s_{x}^{(1)} s_{x}^{(2)} - s_{y}^{(1)} s_{y}^{(2)} \right] + \tilde{K} \left[ s_{x}^{(1)} s_{y}^{(2)} + s_{y}^{(1)} s_{x}^{(2)} \right], \tag{19}$$

where

$$\tilde{\rho}^{2} + \tilde{K}^{2} = J^{2}, \tag{20}$$

with $J$ being the Heisenberg coupling constant in Eq. (16).

By applying the general formulation of the former section to Heisenberg classes, we obtain the following concurrence functions for the corresponding thermal states,

$$C_{s,1}^{\text{HE}} = -\frac{(1 + e^{J/T})}{2Z} < 0,$$

$$C_{s,2}^{\text{HE}} = \frac{e^{J/T} - 3}{2Z}, \tag{21}$$

and

$$C_{s,1}^{\text{AS}} = \frac{e^{J/T} - 3}{2Z},$$

$$C_{s,2}^{\text{AS}} = -\frac{(1 + e^{J/T})}{2Z} < 0, \tag{22}$$

with partition function,

$$Z = 1 + e^{J/T} + 2 \cosh(B/2T). \tag{23}$$

Here we have used the conditions in Eqs. (18) and (20) in the derivations of Eqs. (22)–(23). Note that the swap of the antisymmetric concurrence functions in Eq. (23) compared to its symmetric counterparts in Eq. (22) is what explains the entanglement duality in Heisenberg spin-spin interactions. This duality is associated with coinciding entanglement concurrences,

$$C(\rho_{T,s}^{\text{HE}}) = \max \left\{ \frac{e^{J/T} - 3}{2Z}, 0 \right\} = C(\rho_{T,as}^{\text{HE}}), \tag{24}$$

for both symmetric and antisymmetric Heisenberg thermal states. Equation (24) defines the critical temperature (that is independent of the external magnetic field),

$$T_{c}^{\text{HE}} = \sqrt{J^{2} + D^{2}} / \ln 3 = J / \ln 3 \approx 0.91J. \tag{25}$$

above which as shown in Fig. 3, the thermal states $\rho_{T,s}^{\text{HE}}$ and $\rho_{T,as}^{\text{HE}}$ cease to be entangled. The same critical temperature has been obtained in Ref. [15] for antiferromagnetic Heisenberg model given in Eq. (16). Nonetheless, our analysis shows that this critical temperature indeed holds for a wider class of spin-spin interactions.

The entanglement duality for the Heisenberg interaction is identified mainly by the toric characteristic equations given in Eqs. (18) and (20). As illustrated in Fig. 3, these equations foliate the corresponding dual parameter spaces $(J', D')$ in the $(r, K)$ plane of radii specified by the Heisenberg exchange parameter $J$. Each radius identifies dual circles representing dual-symmetric and -antisymmetric classes associated with the Heisenberg spin-spin interaction. Moreover, all spin-spin interaction Hamiltonians in given dual topological classes obey the same critical temperature, given in Eq. (25).

As another example, Fig. 4 illustrates the classification of the XY interaction described by the Hamiltonian,

$$H_{XY} = (1 + r)x_{x}^{(1)}x_{x}^{(2)} + (1 - r)y_{y}^{(1)}y_{y}^{(2)} + \frac{B}{2} [s_{z}^{(1)} + s_{z}^{(2)}], \tag{26}$$

(with superscript XY) into dual toric entanglement classes. Here $r \in [0, 1]$ is the anisotropy parameter controlling the cylindrical asymmetry of the spin-spin interaction. The XY model given in Eq. (26) defines interactions from the isotropic limit $r = 0$ with additional symmetry $[H_{XY}, s_{z}] = 0$ to the opposite limit $r = 1$, which corresponds to the Ising type of interactions.

The XY interaction given in Eq. (26) represents a symmetric class of dimers. Following Eqs. (12) and (13), the associated general symmetric and dual-antisymmetric
We obtain the following concurrence functions for the XY classes of thermal states,

\[ C^{XY}_{s;1} = \frac{1}{2} \left[ \frac{r \sinh \left( \frac{\sqrt{B^2 + r^2}}{2T} \right)}{\sqrt{B^2 + r^2}} - \cosh \left( \frac{1}{2T} \right) \right] = C^{XY}_{as;1}, \]

\[ C^{XY}_{s;2} = \frac{1}{2} \left[ \sinh \left( \frac{1}{2T} \right) - \frac{r^2 \sinh^2 \left( \frac{\sqrt{B^2 + r^2}}{2T} \right)}{B^2 + r^2} \right] = C^{XY}_{as;2}, \]  

with partition function \( Z = 2 \cosh(\frac{1}{2T}) + 2 \cosh(\frac{\sqrt{B^2 + r^2}}{2T}) \).

For all \( r \neq 0 \), Eq. (31) derives a magnetic-field-dependent critical temperature given implicitly by

\[ \max \left( C^{XY}_{s;1}, C^{XY}_{s;2} \right) = \max \left( C^{XY}_{as;1}, C^{XY}_{as;2} \right) = 0. \]

Figure 4 illustrates critical temperatures as functions of the magnetic field for some values of \( r \).

IV. CONCLUSIONS

In conclusion, we have demonstrated an entanglement duality in a wide class of physically important spin-spin interaction dimer models. This is performed by analyzing an entanglement transition of thermal states on the temperature-magnetic-field plane. The entanglement analysis allows to foliate the coupling parameter space into a dual-pair of symmetric and antisymmetric toric entanglement classes. This classification is an indication of the topological signature of quantum entanglement in the sense that quantum entanglement is consistent up to topological classifications. The analysis shows the stability of entanglement against parameter changes within a broader topological domain, which could be relevant for the processing of quantum information. We hope the present results can contribute to a deeper understanding of the hidden aspects of the concept of quantum entanglement, and that it is an inspiration to works in nanomagnetism where magnetic nanosized objects of the type investigated here are under focus.

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